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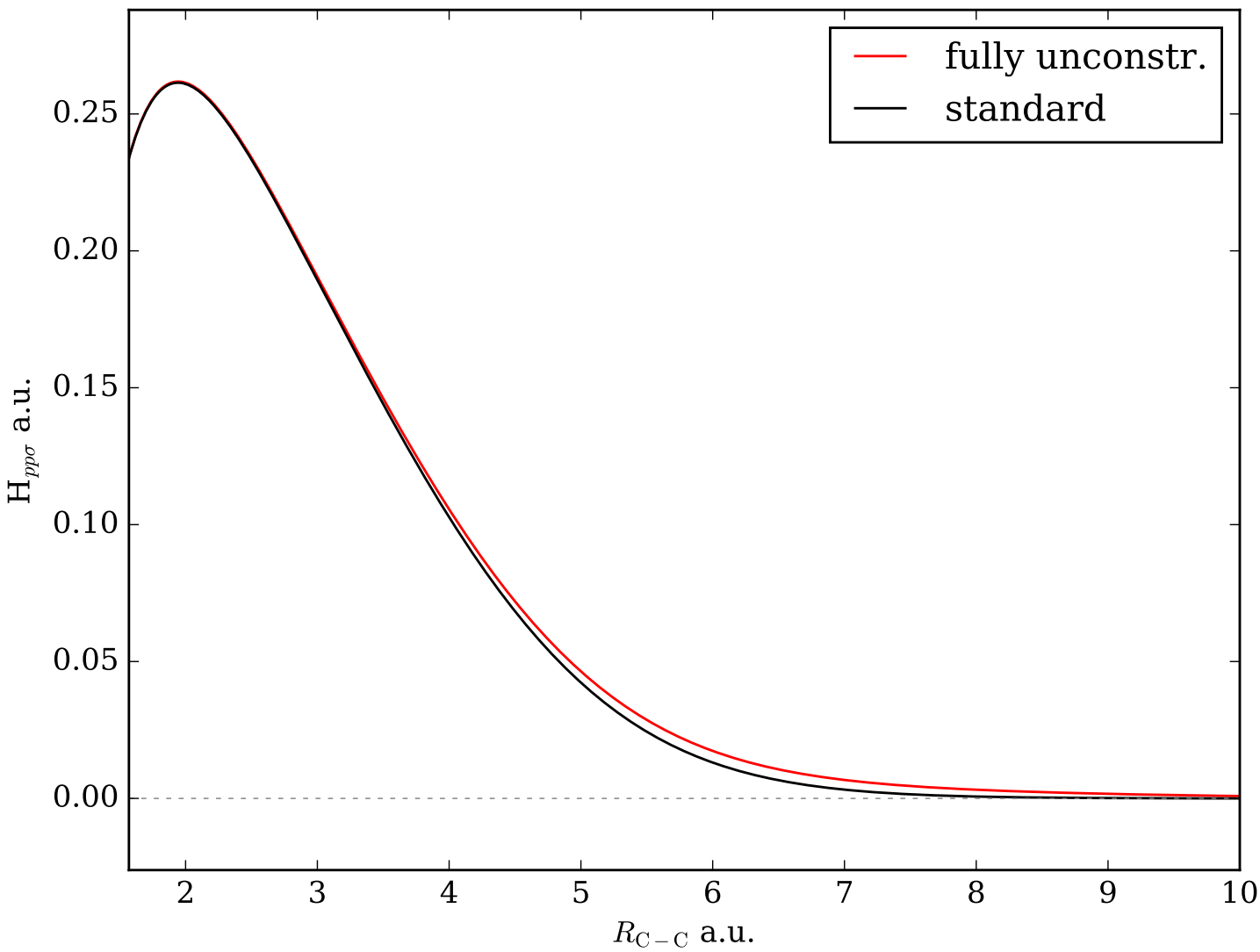
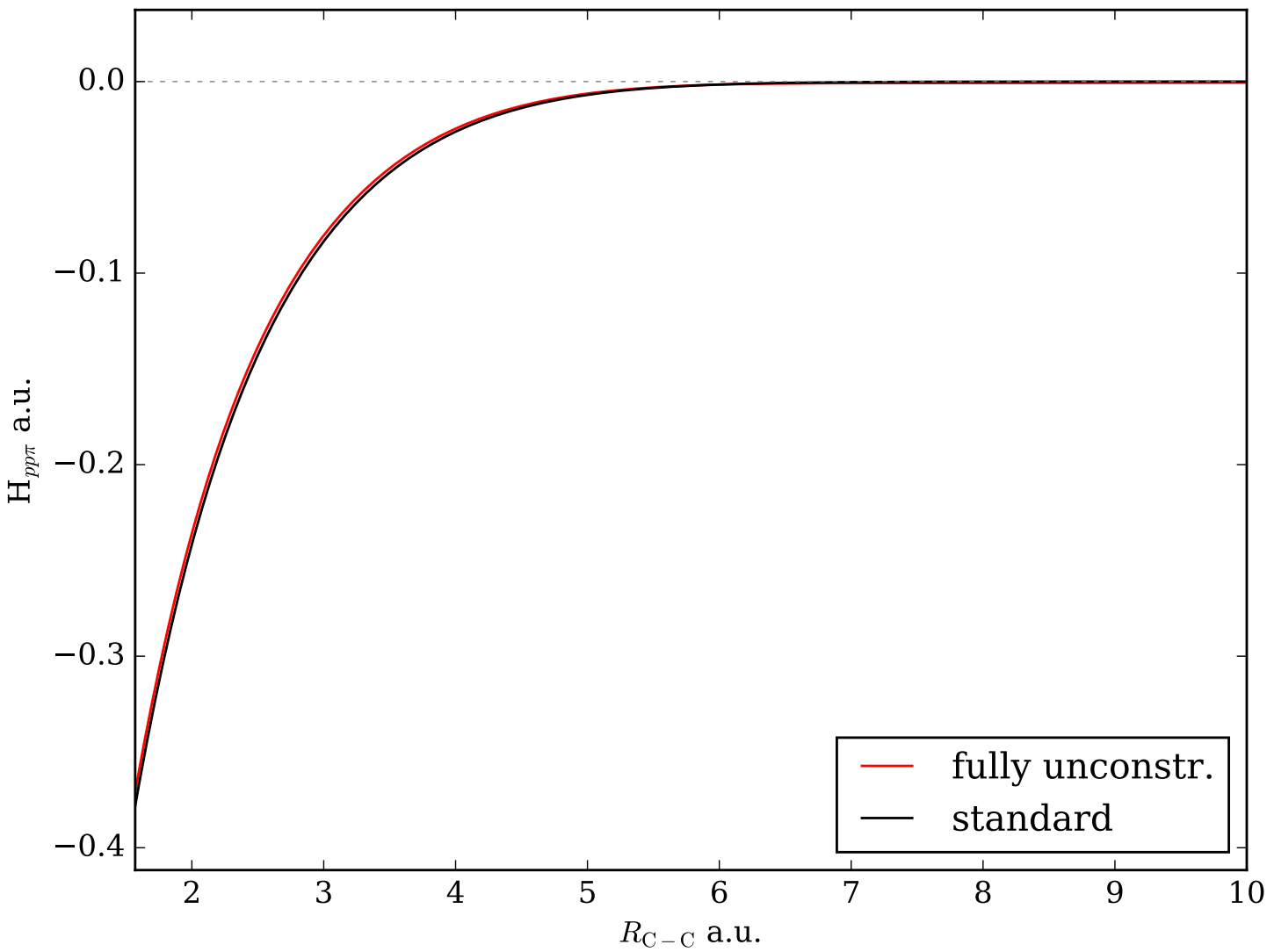
1 C-C

1.1 Electronic

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$H_{pp\pi}$ a.u.
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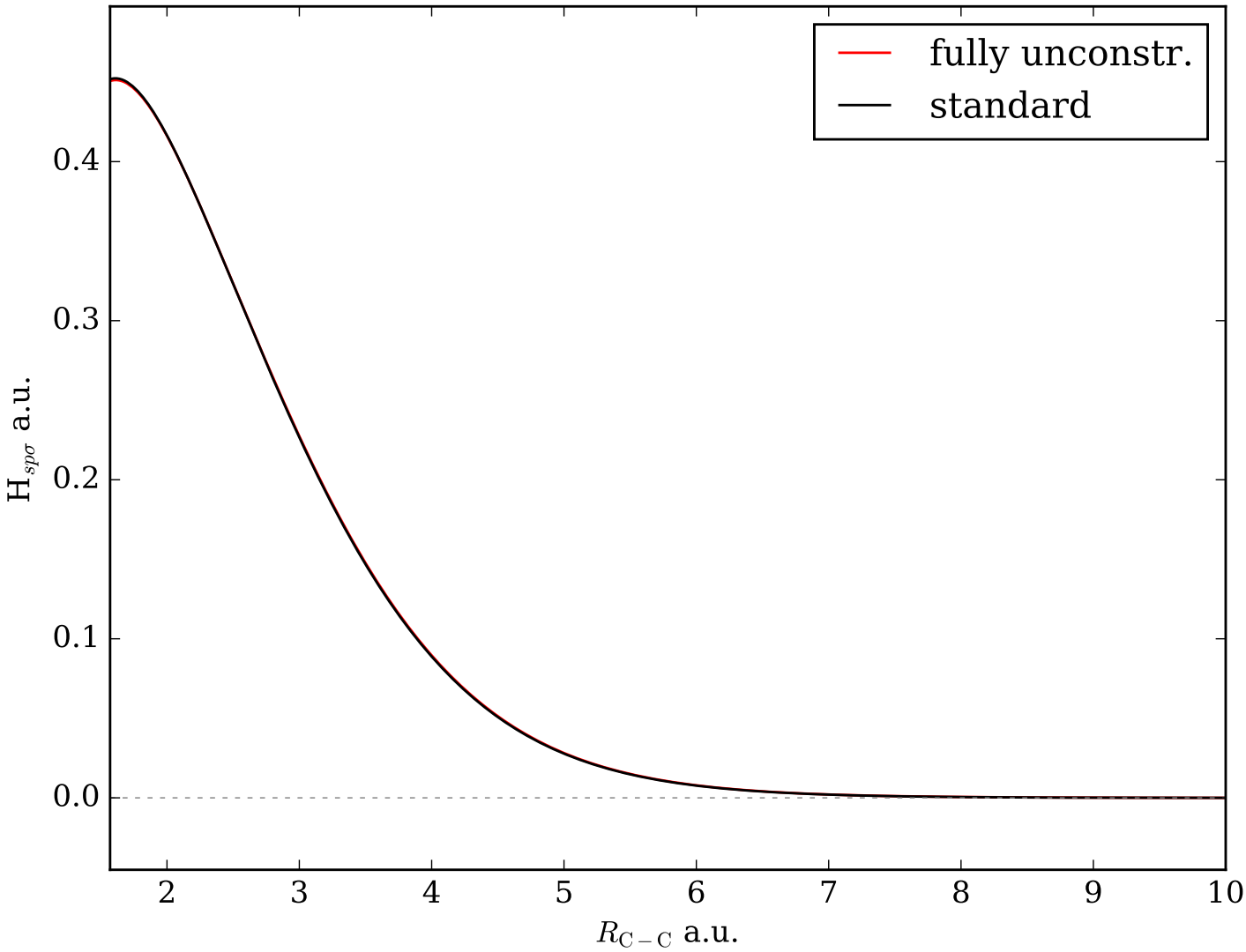
3
4
5
6
7
8
9
10
R_{C-C} a.u.
fully unconstr.
standard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9
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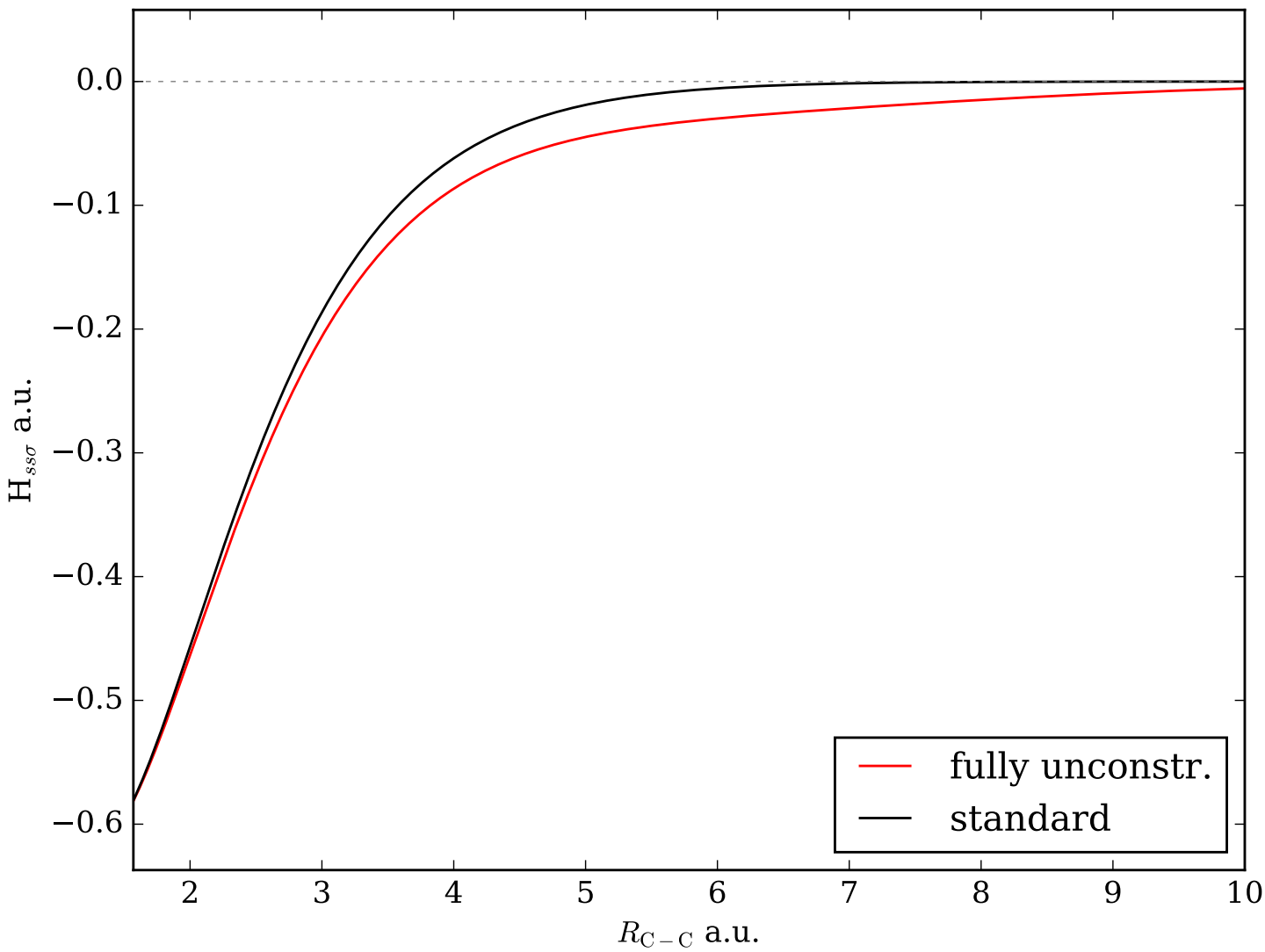
R_{C-C} a.u.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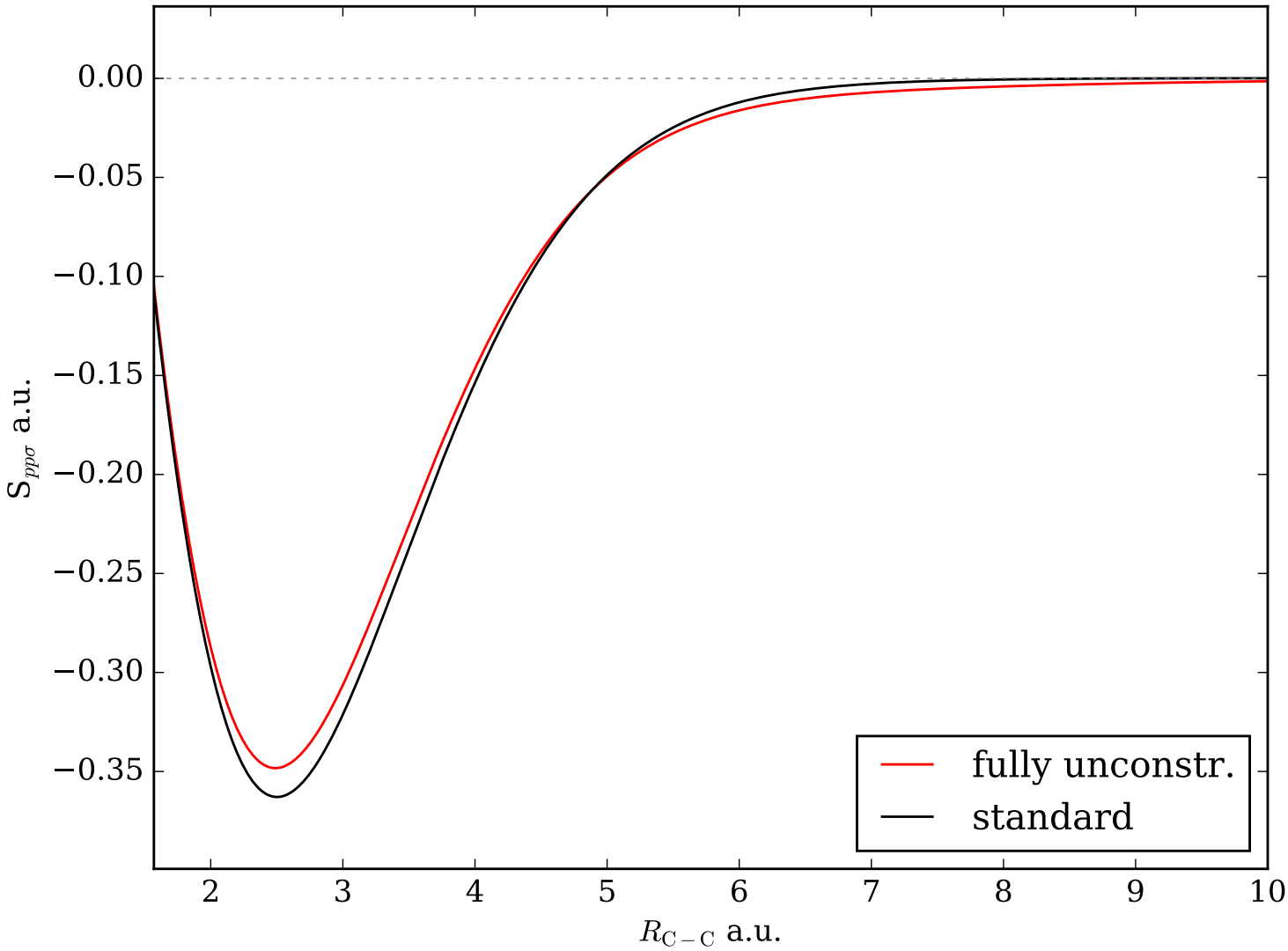
fully unconstr.
standard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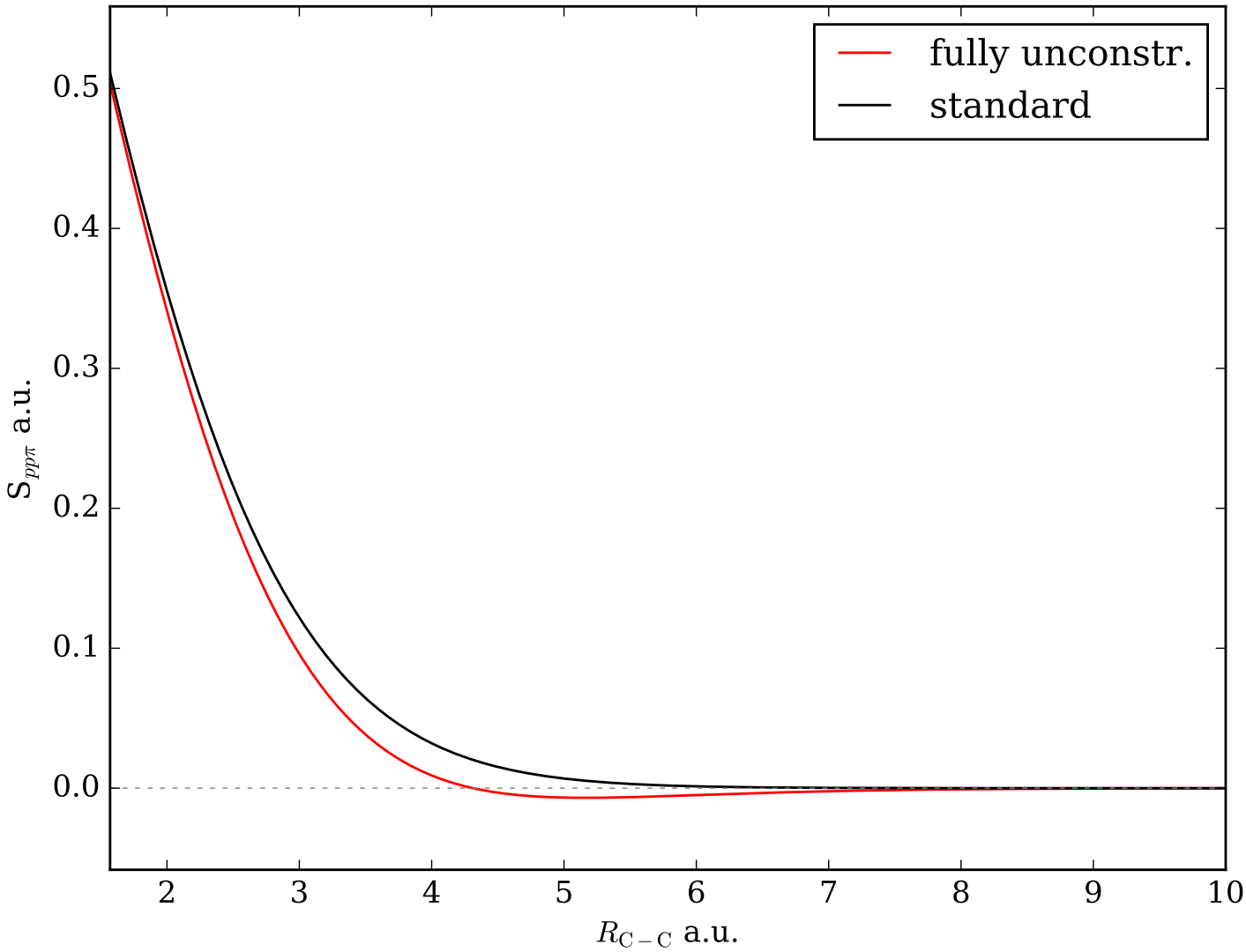
$R_{\mathrm{C-C}}$ a.u.
fully unconstr.
standard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7
8
9
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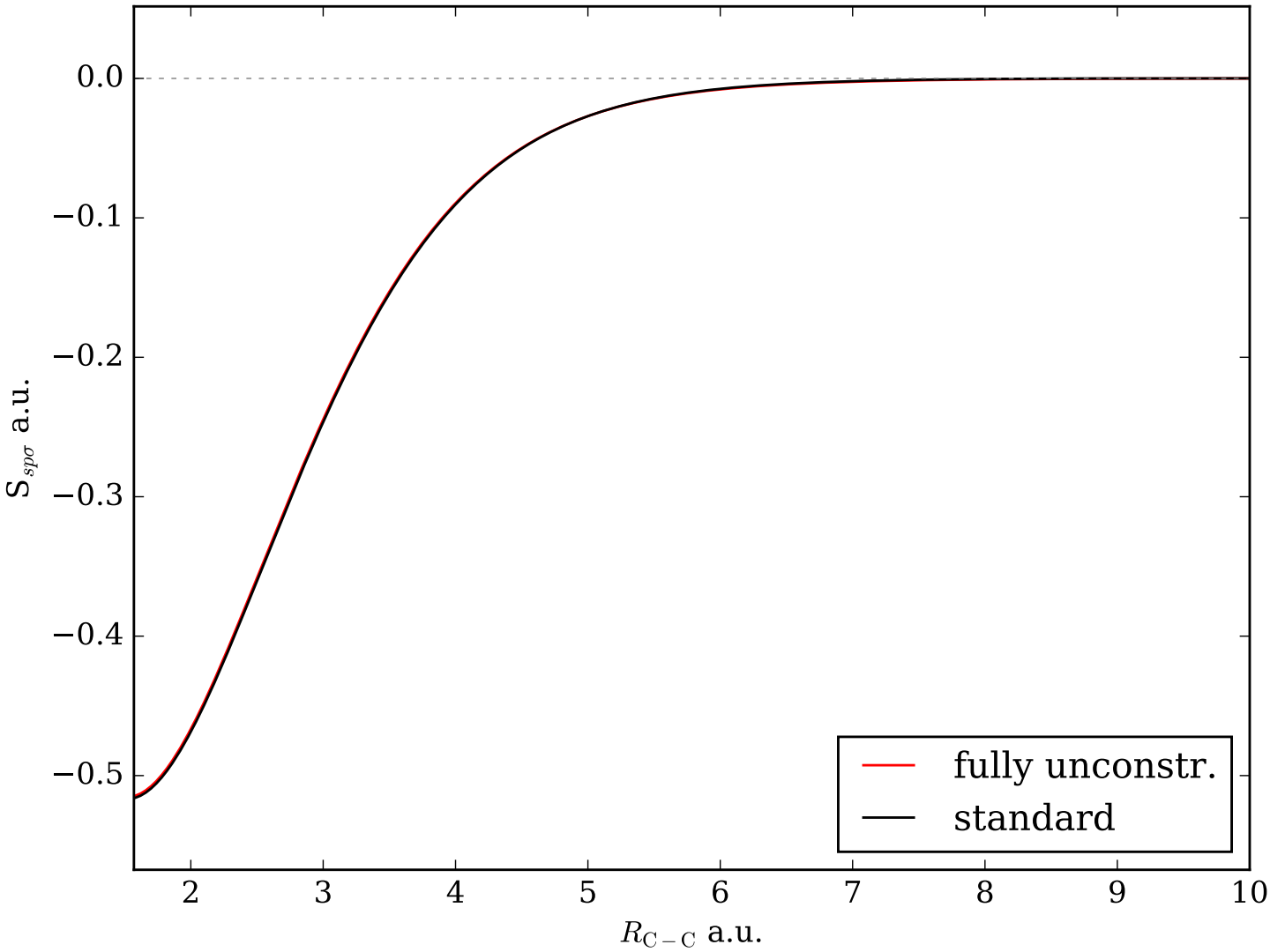
$R_{\mathrm{C-C}}$ a.u.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$S_{sp\sigma}$ a.u.
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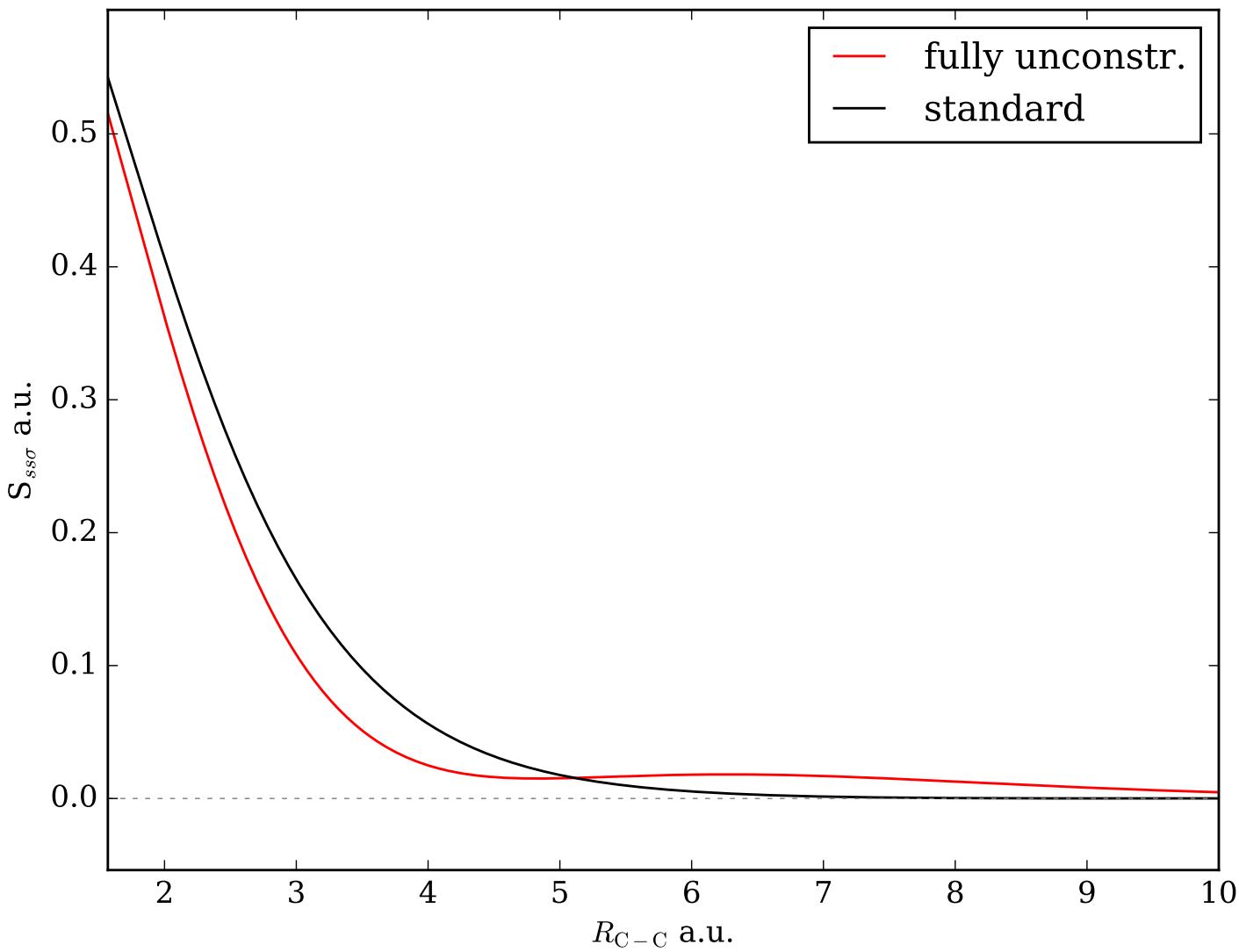
7
8
9
10
$R_{\mathrm{C-C}}$ a.u.
fully unconstr.
standard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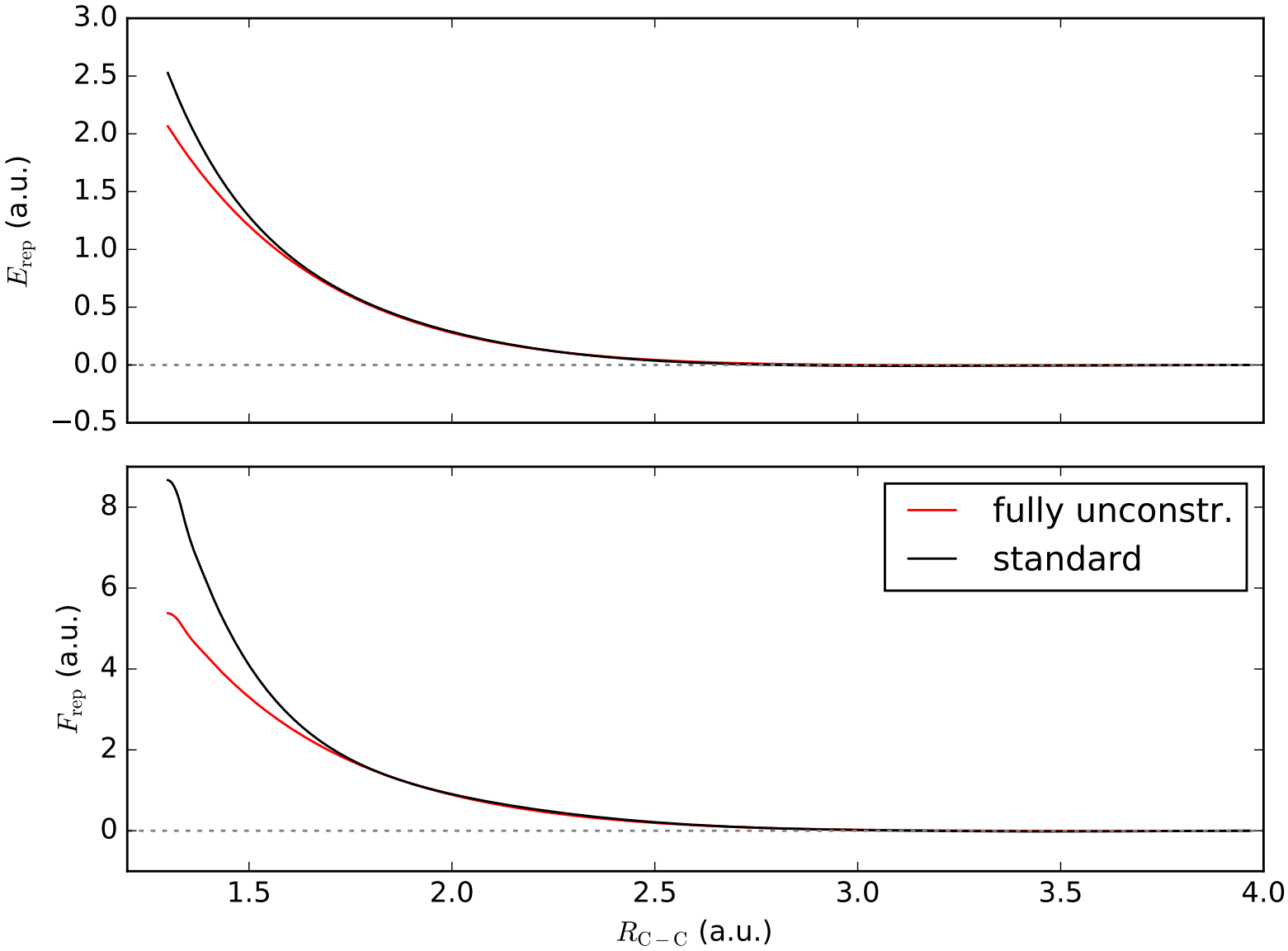
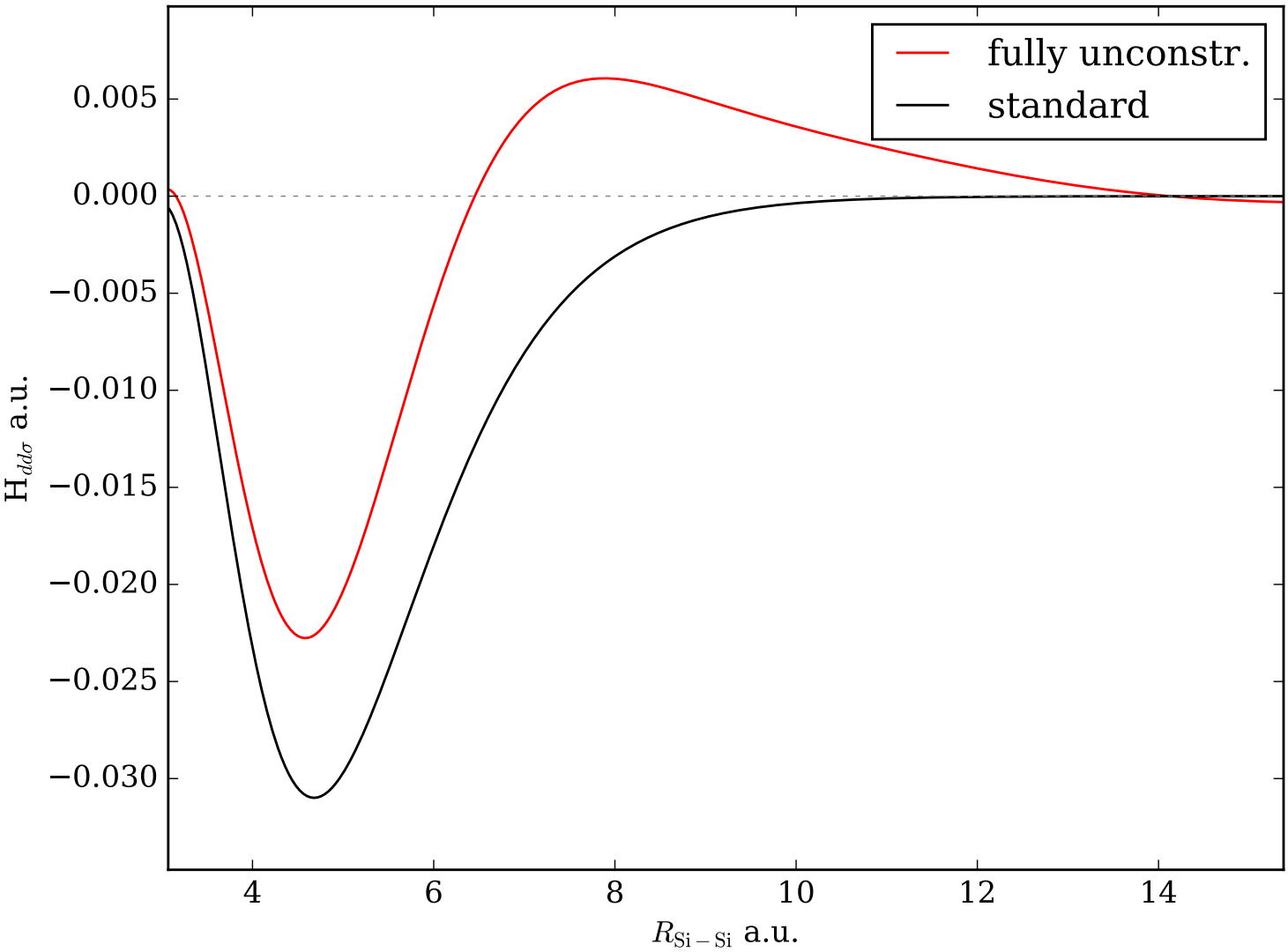
0.0
$S_{ss\sigma}$ a.u.
2
3
4
5
6
7
8
9
10
$R_{\mathrm{C-C}}$ a.u.

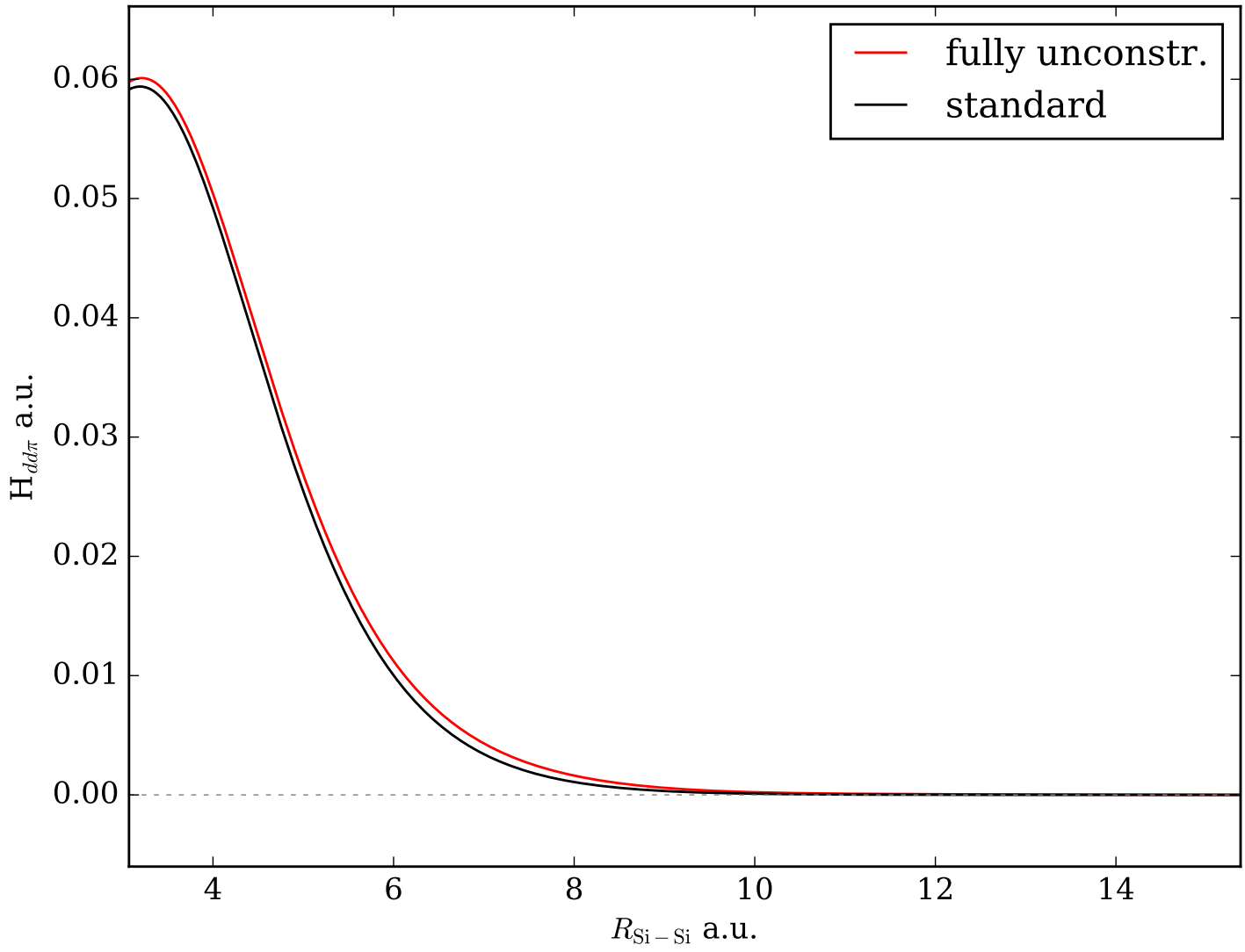
1.2 Repulsive



2 Si-Si

2.1 Electronic




fully unconstr.
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0.04
0.03
0.02
0.01
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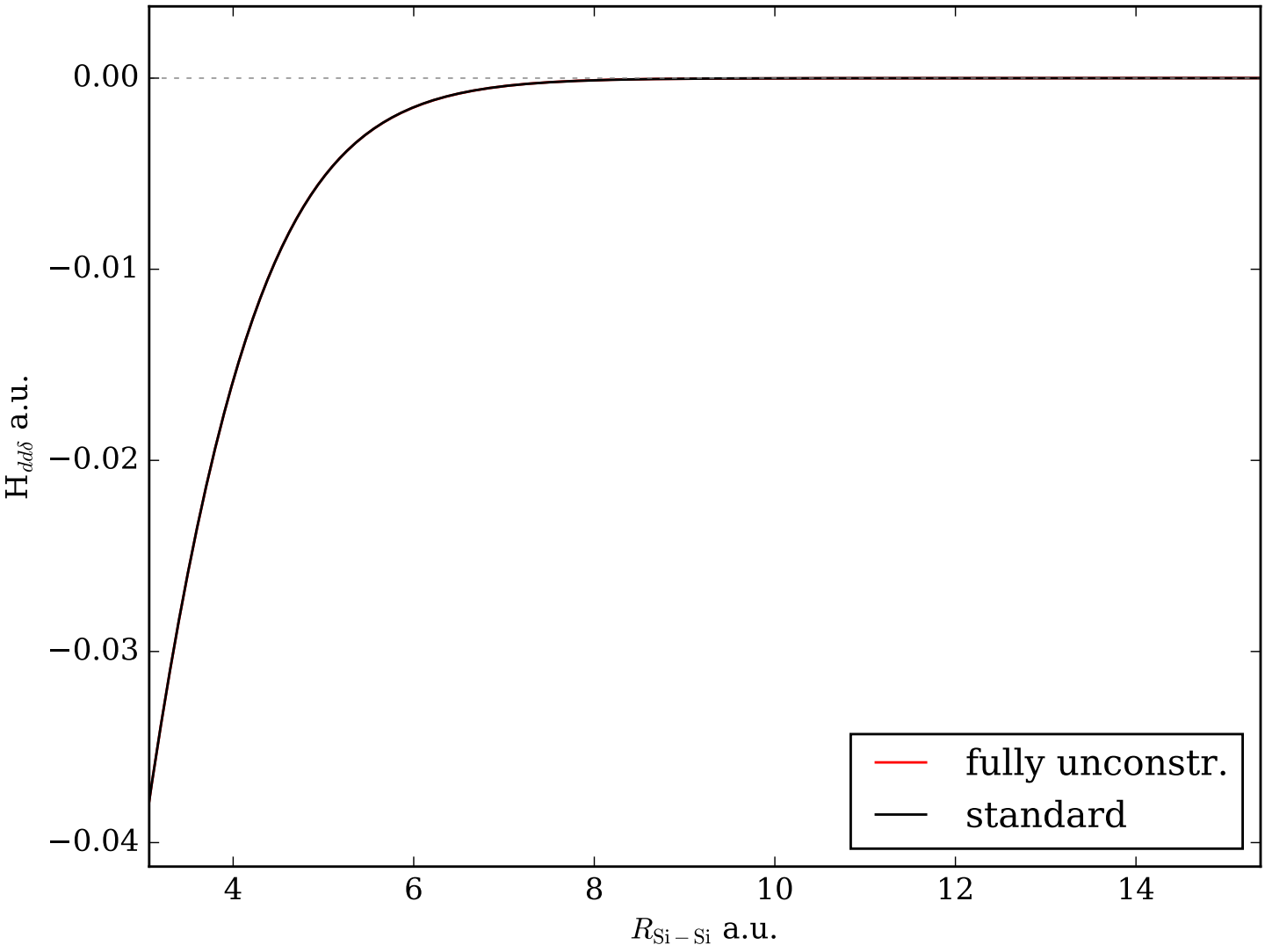
6
8
10
12
14
$R_{\mathrm{Si-Si}}$ a.u.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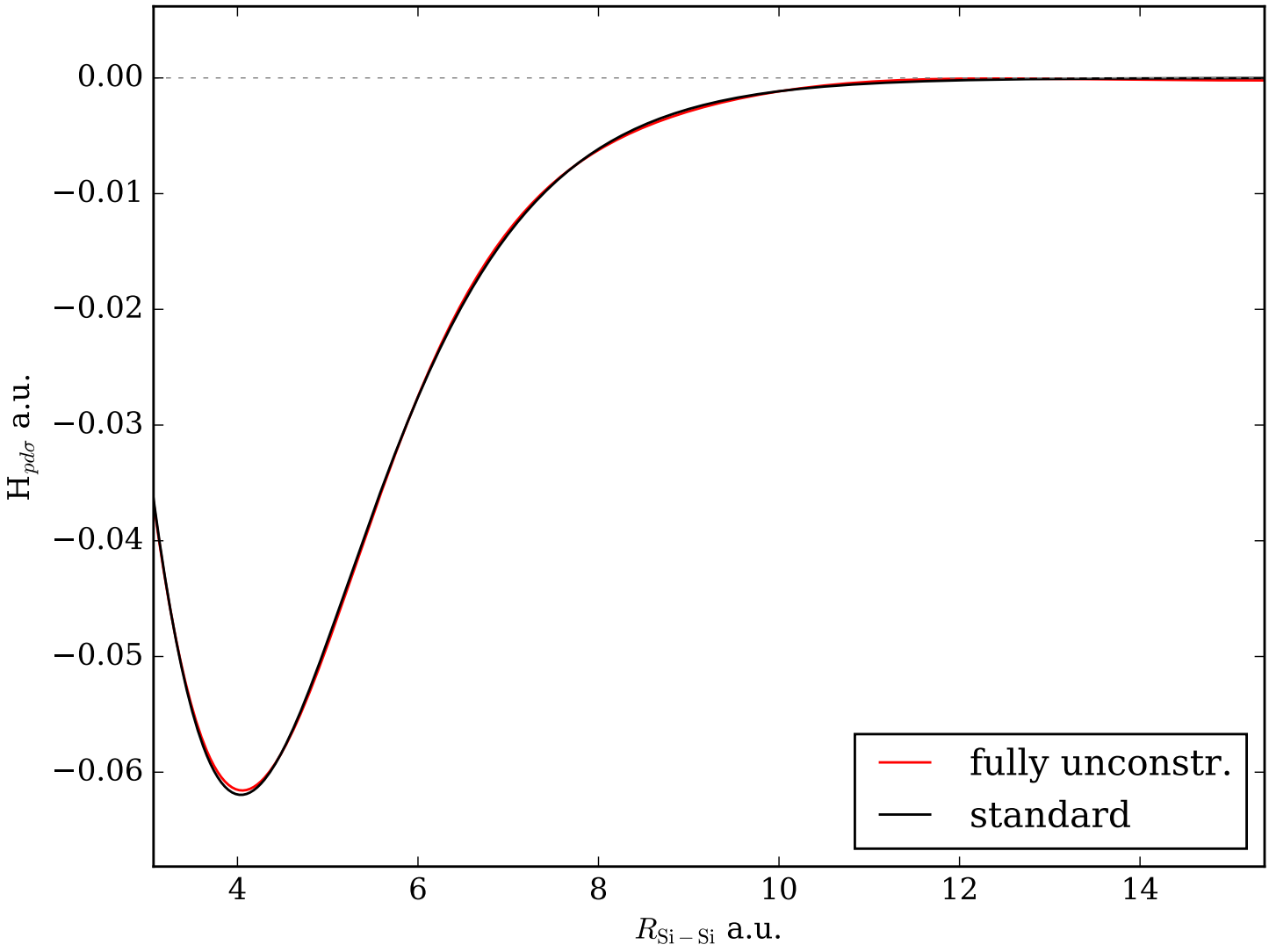
6
8
10
12
14
$R_{\mathrm{Si-Si}}$ a.u.
fully unconstr.
standard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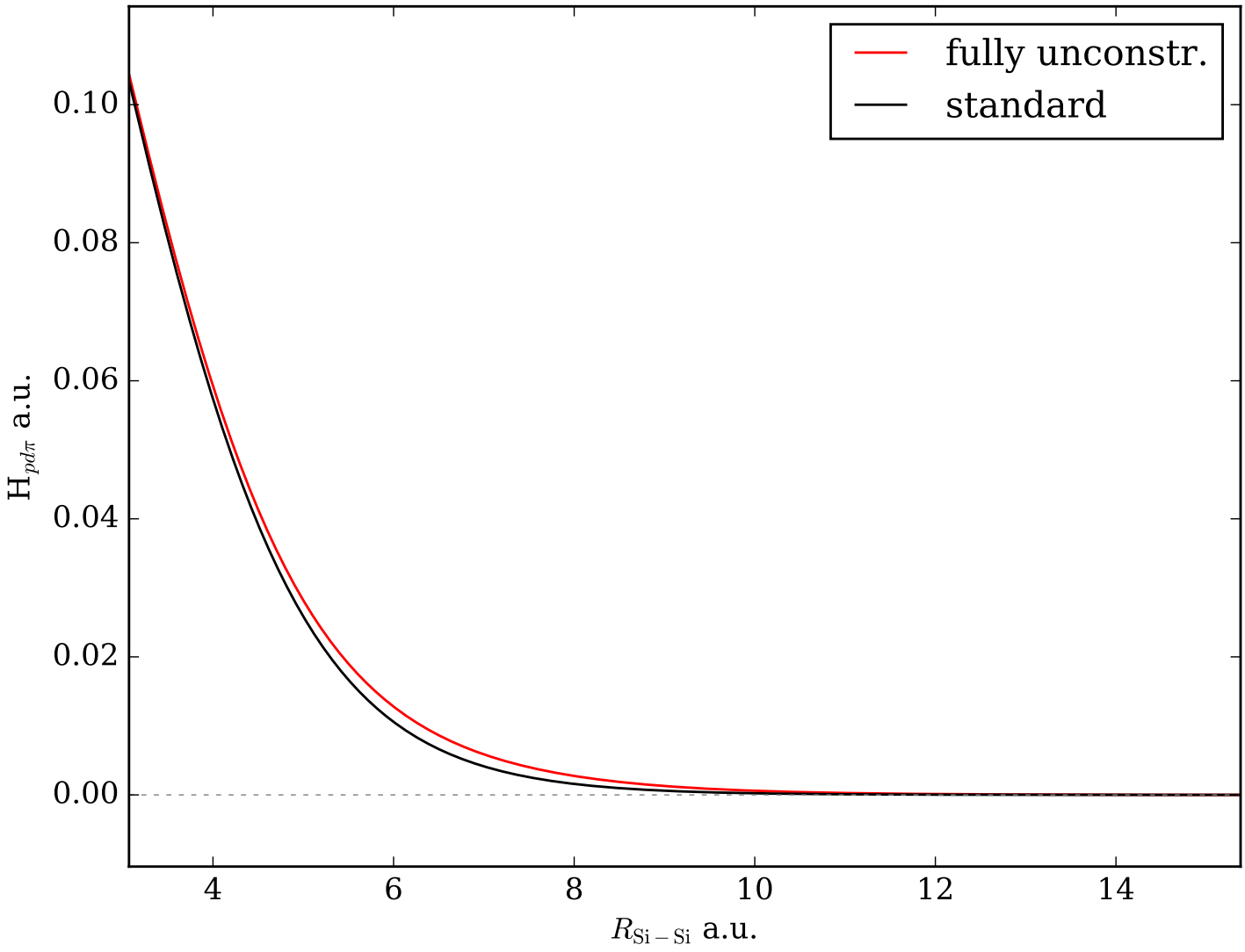
6
8
10
12
14
$R_{\mathrm{Si-Si}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
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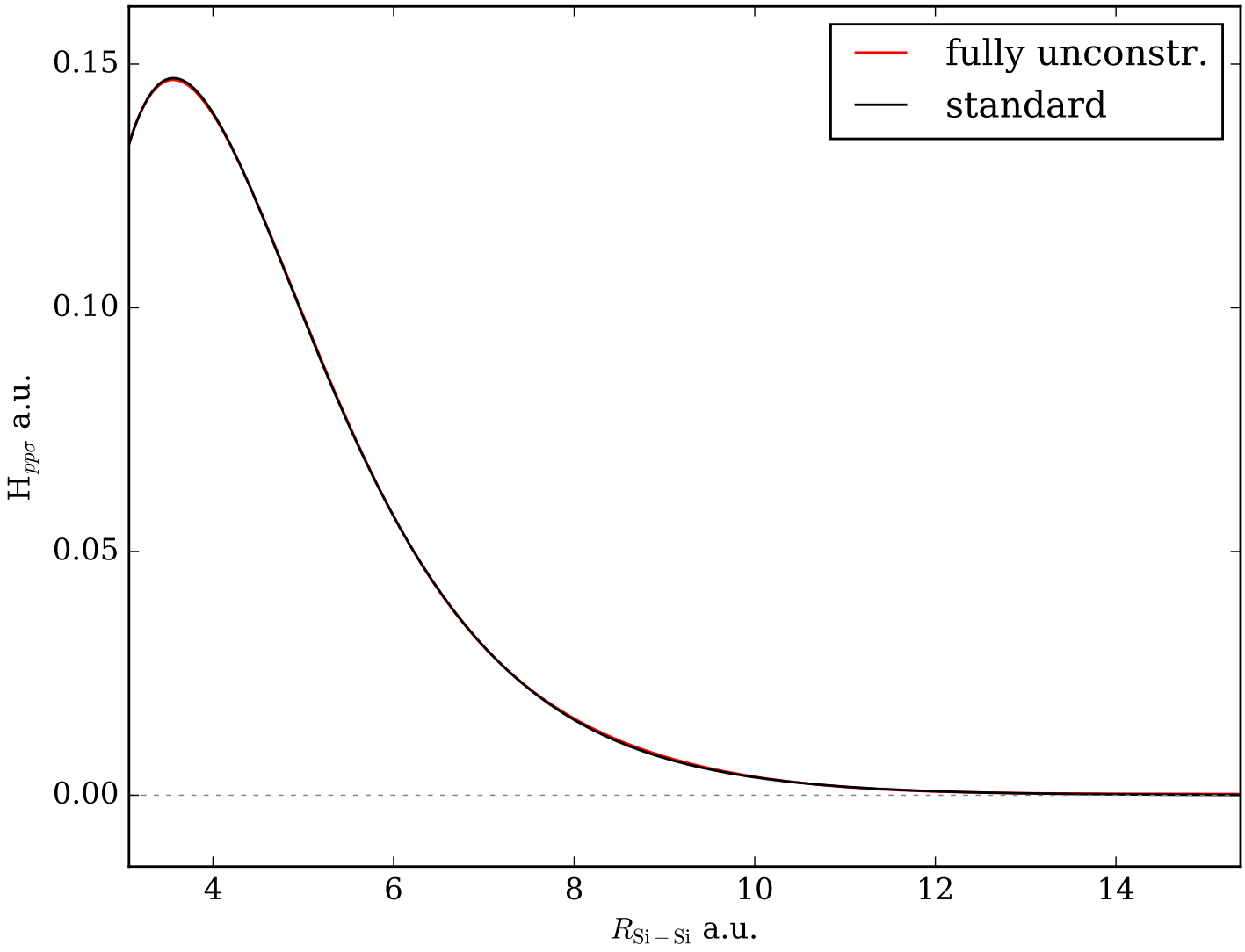
0.06
0.04
0.02
0.00
$H_{pd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Si}}$ a.u.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standard
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$H_{pp\sigma}$ a.u.
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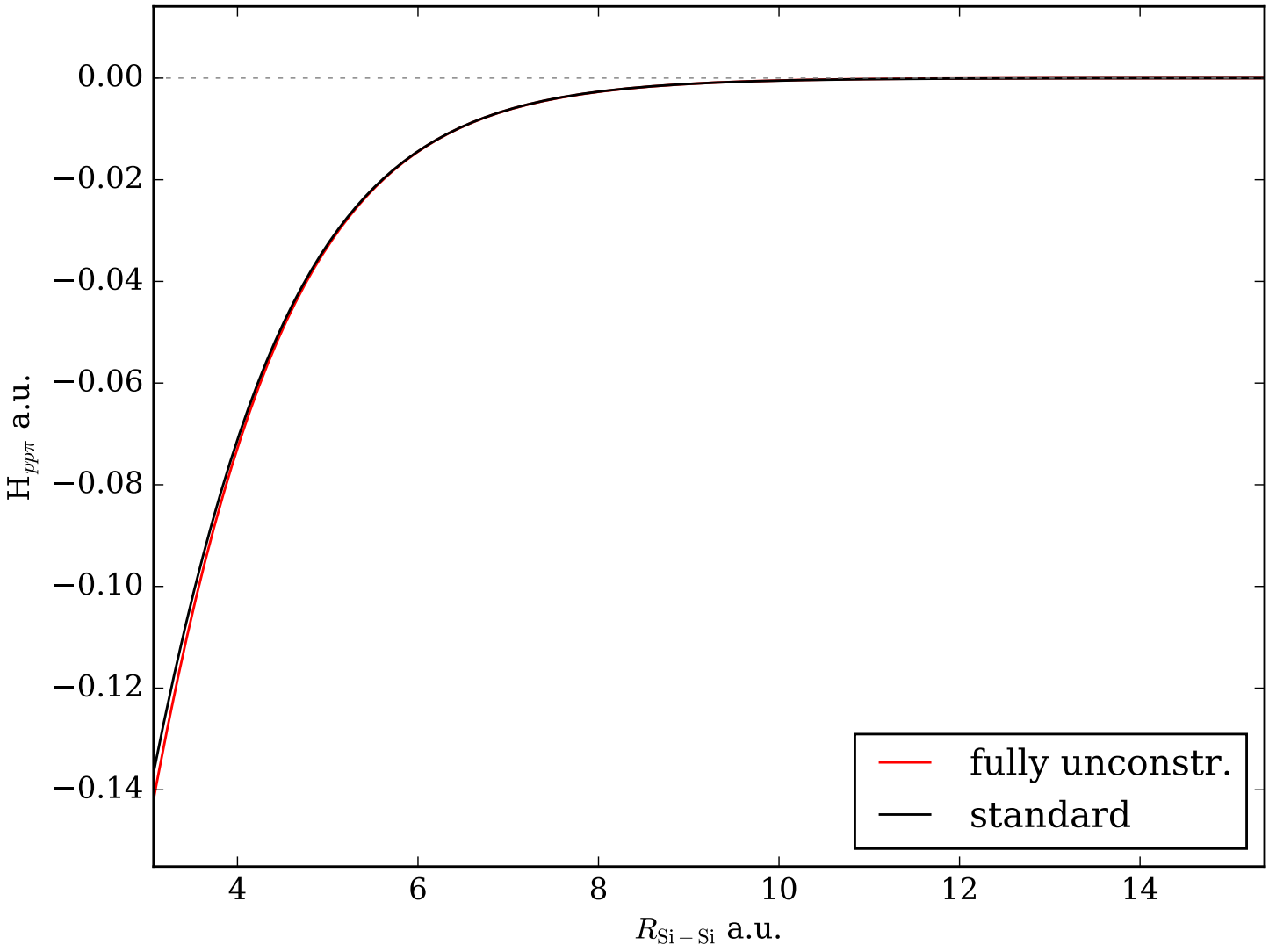
10
12
14
$R_{\mathrm{Si-Si}}$ a.u.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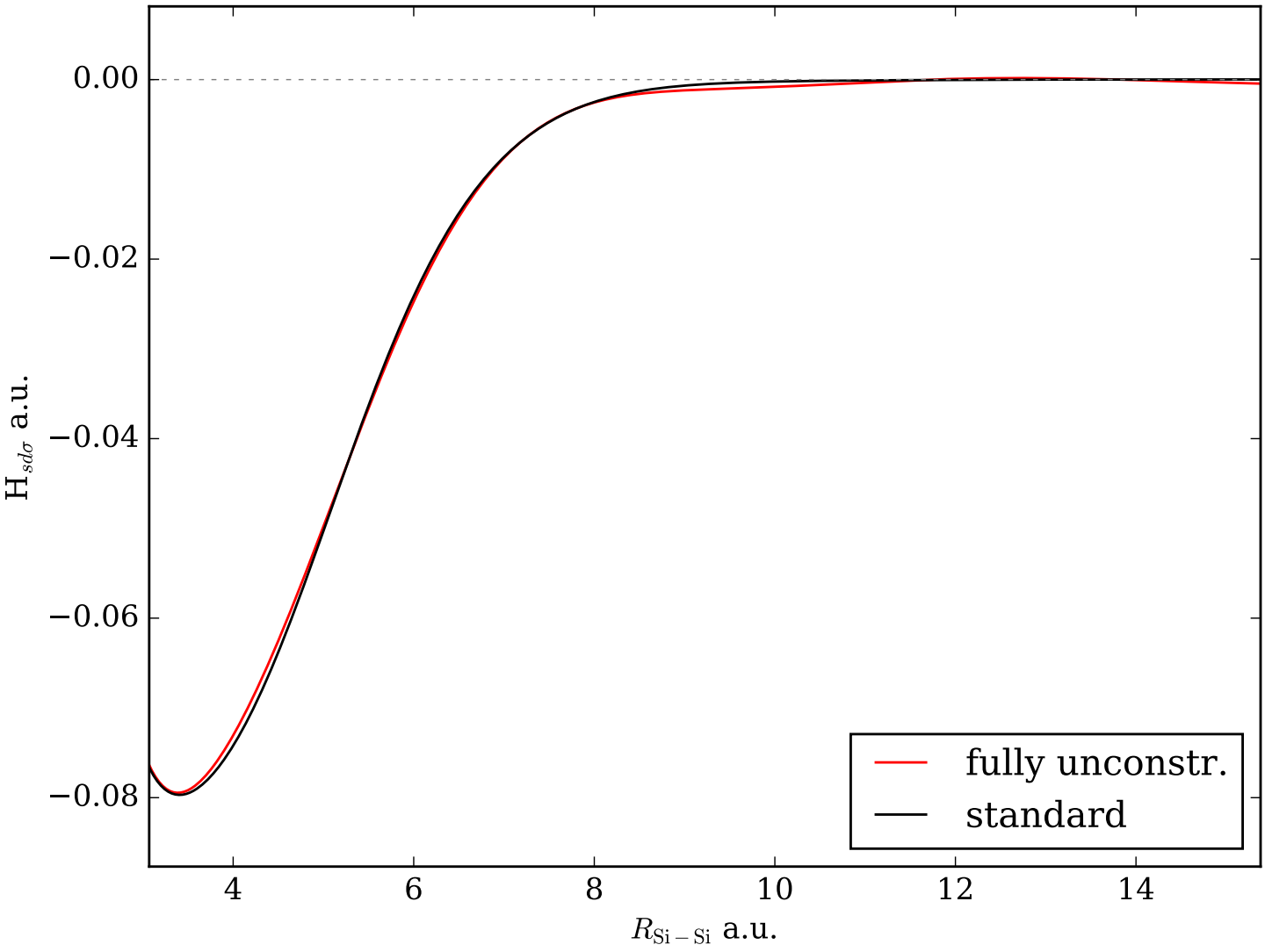
6
8
10
12
14
$R_{\mathrm{Si-Si}}$ a.u.
fully unconstr.
standard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10
12
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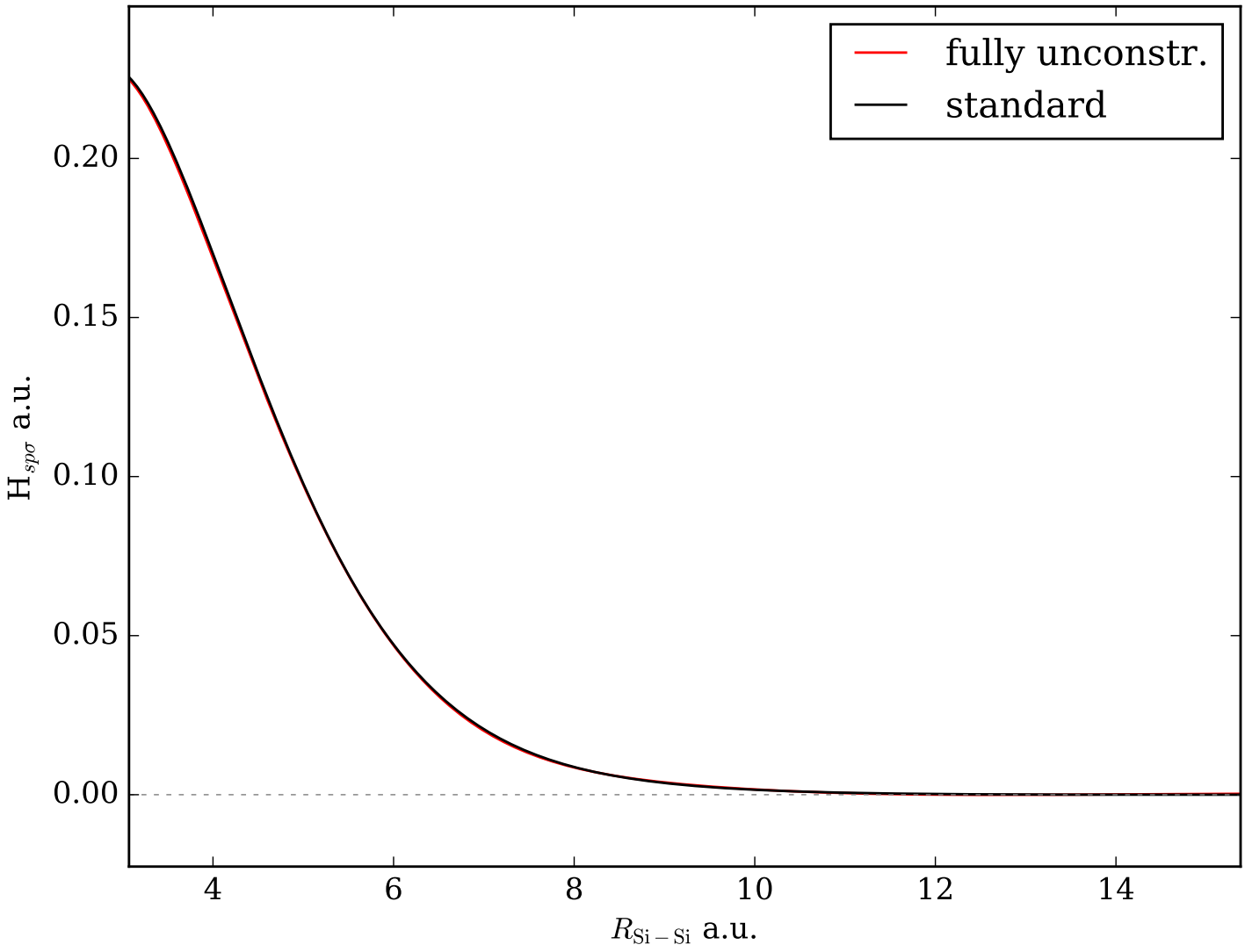
$R_{\mathrm{Si-Si}}$ a.u.
fully unconstr.
standard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$H_{sp\sigma}$ a.u.
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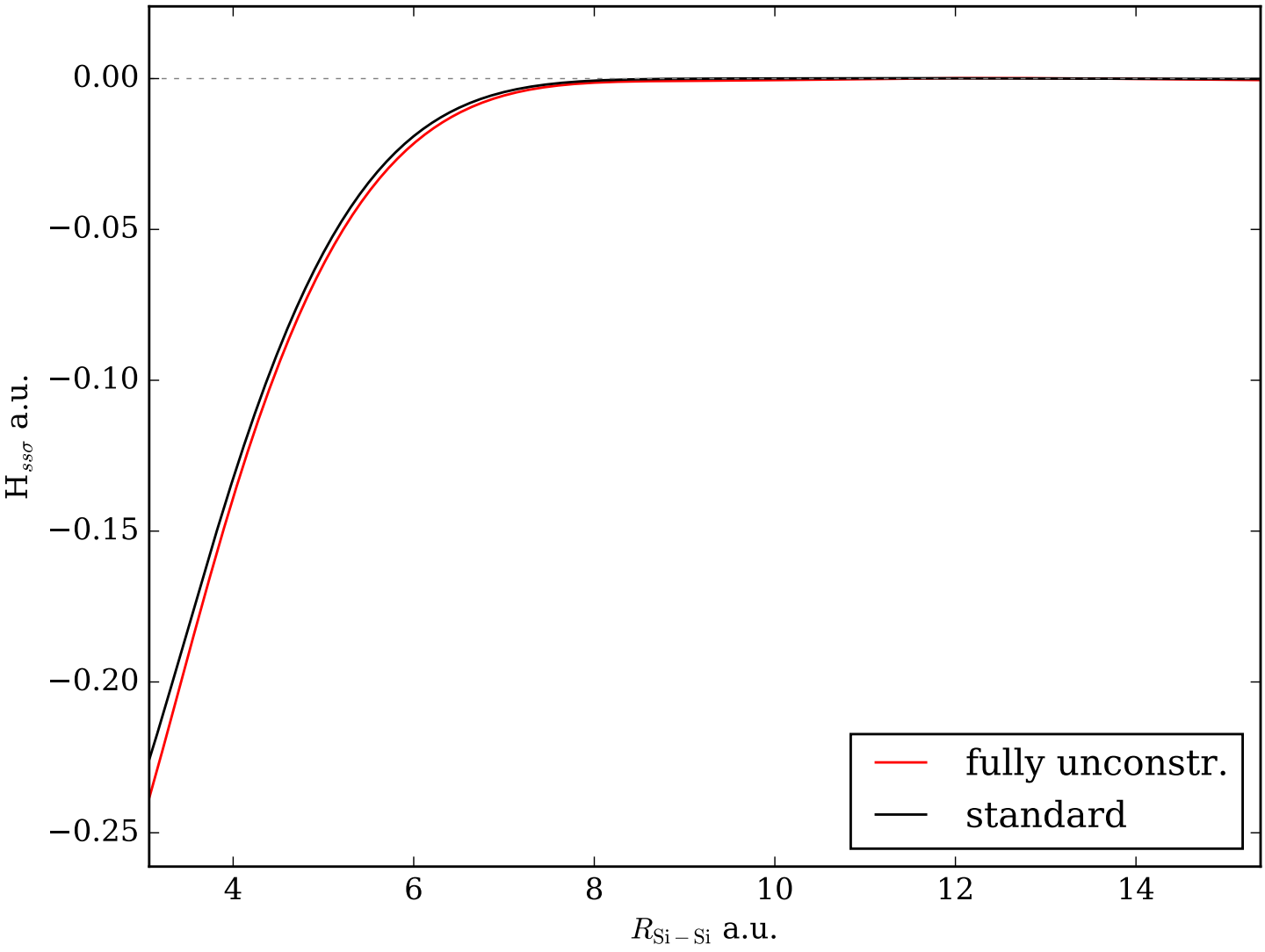
12
14
$R_{\mathrm{Si-Si}}$ a.u.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−0.15
−0.20
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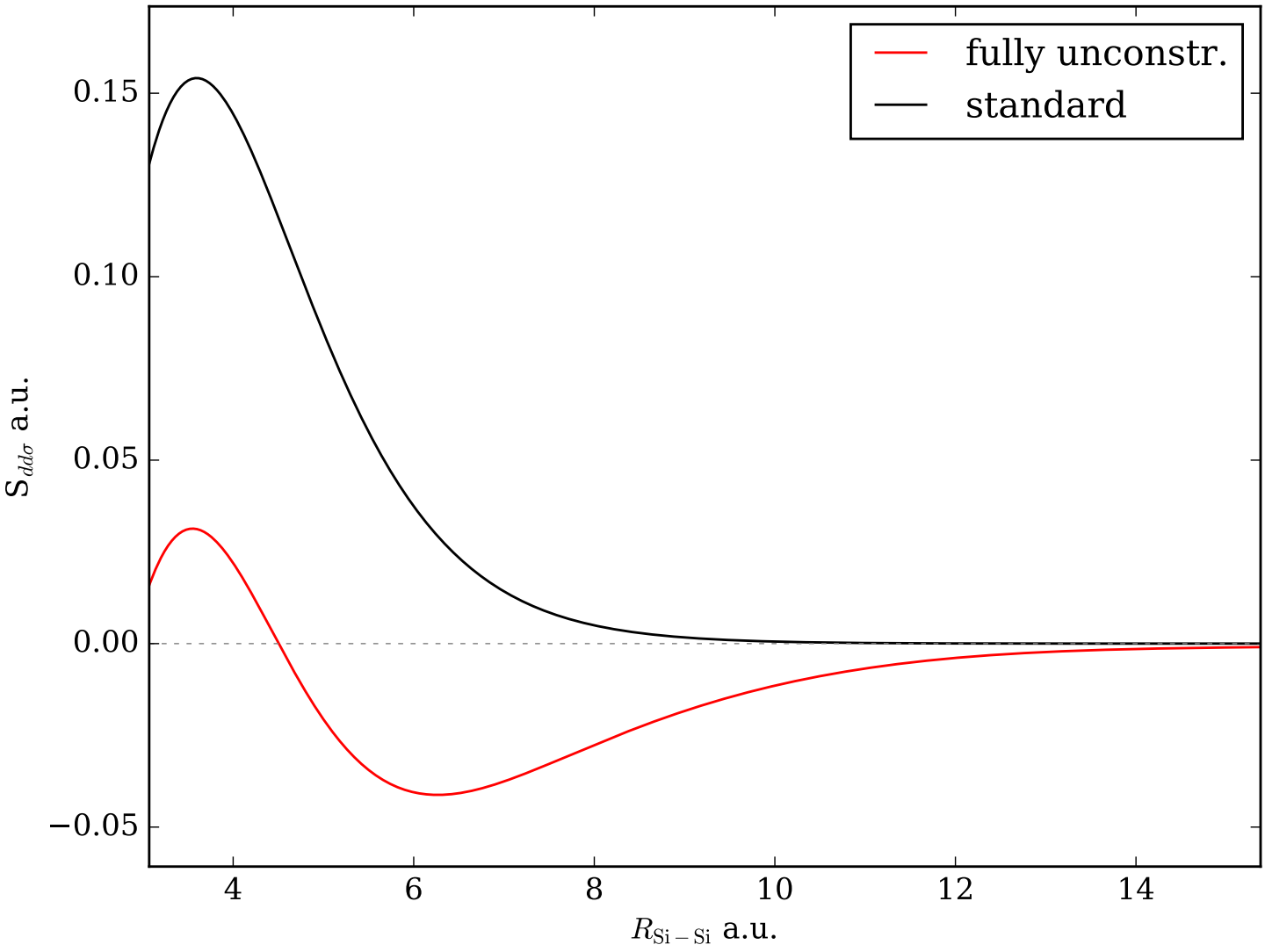
$H_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Si}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
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0.10
0.05
0.00
−0.05
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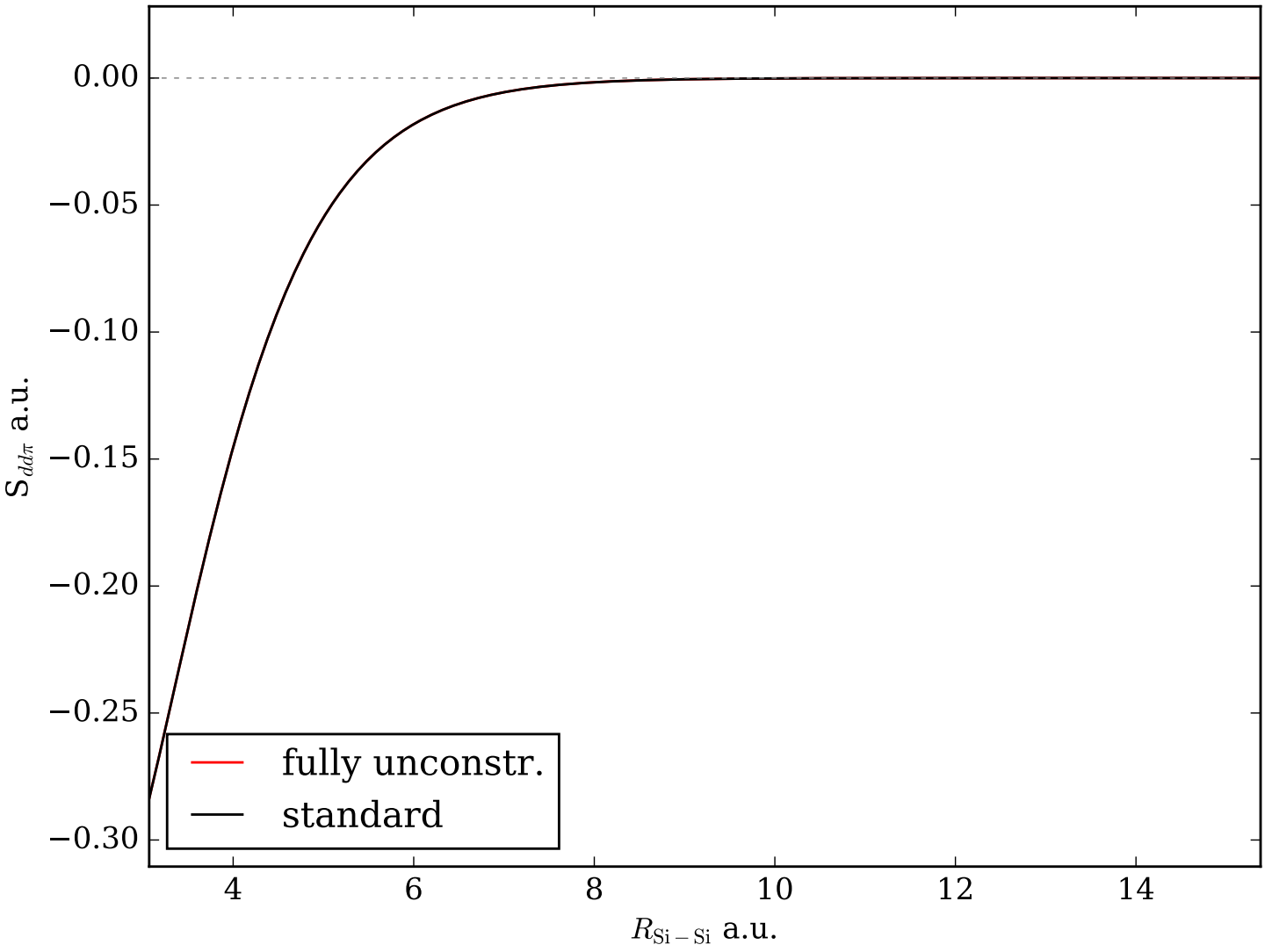
8
10
12
14
$S_{dd\sigma}$ a.u.
$R_{\mathrm{Si-Si}}$ a.u.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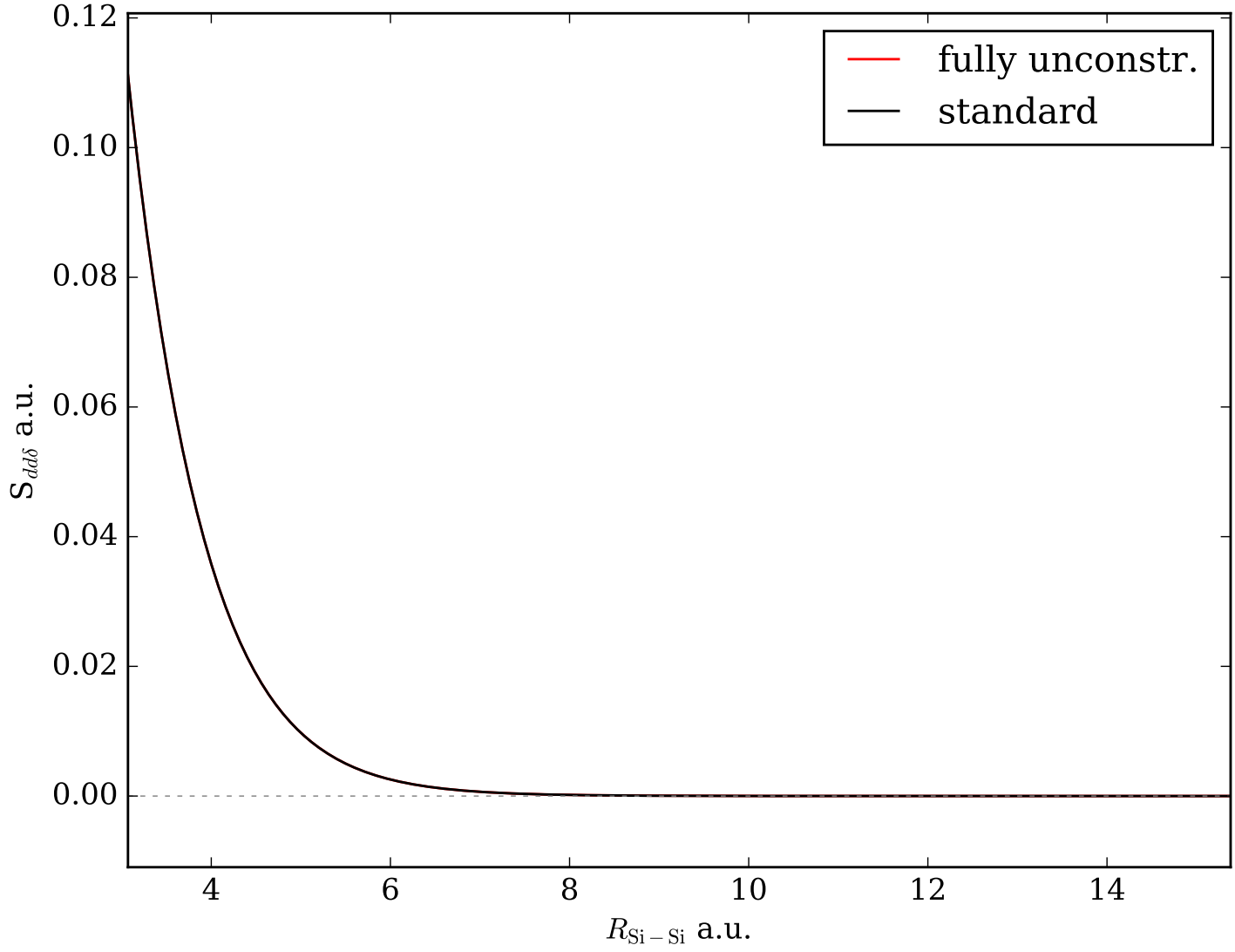
6
8
10
12
14
$R_{\mathrm{Si-Si}}$ a.u.
fully unconstr.
standard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10
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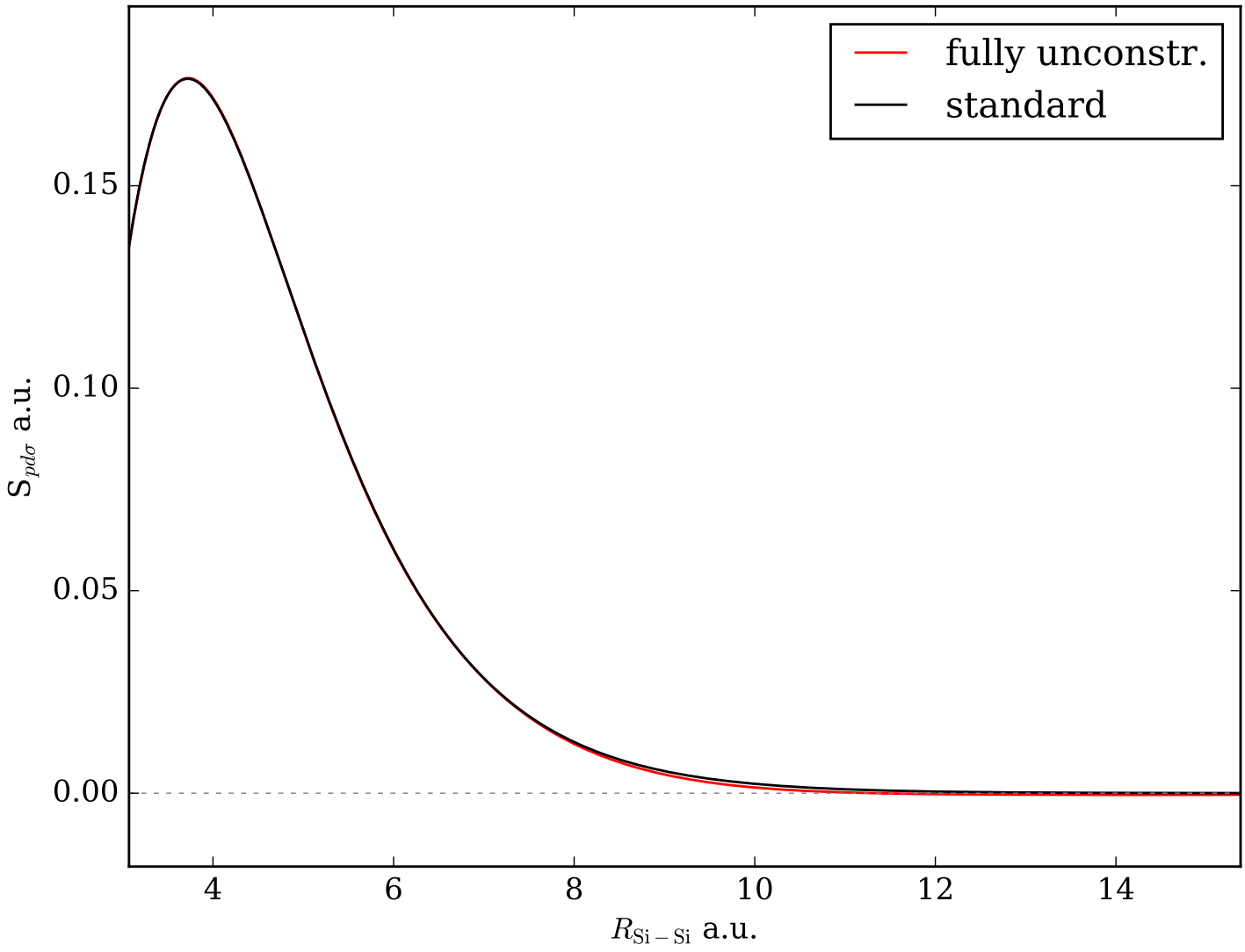
14
$R_{\mathrm{Si-Si}}$ a.u.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standard
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0.05
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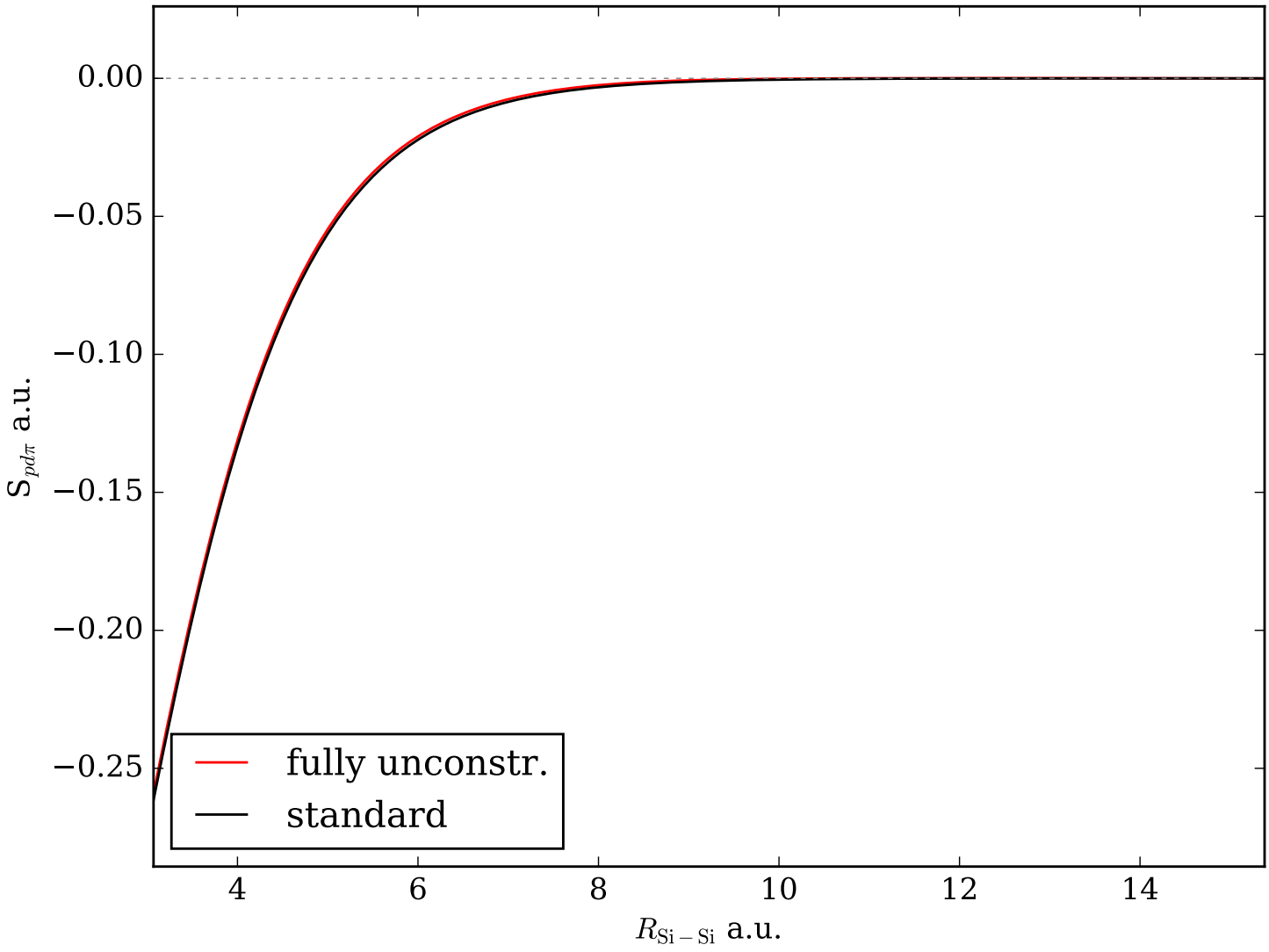
4
6
8
10
12
14
$R_{\mathrm{Si-Si}}$ a.u.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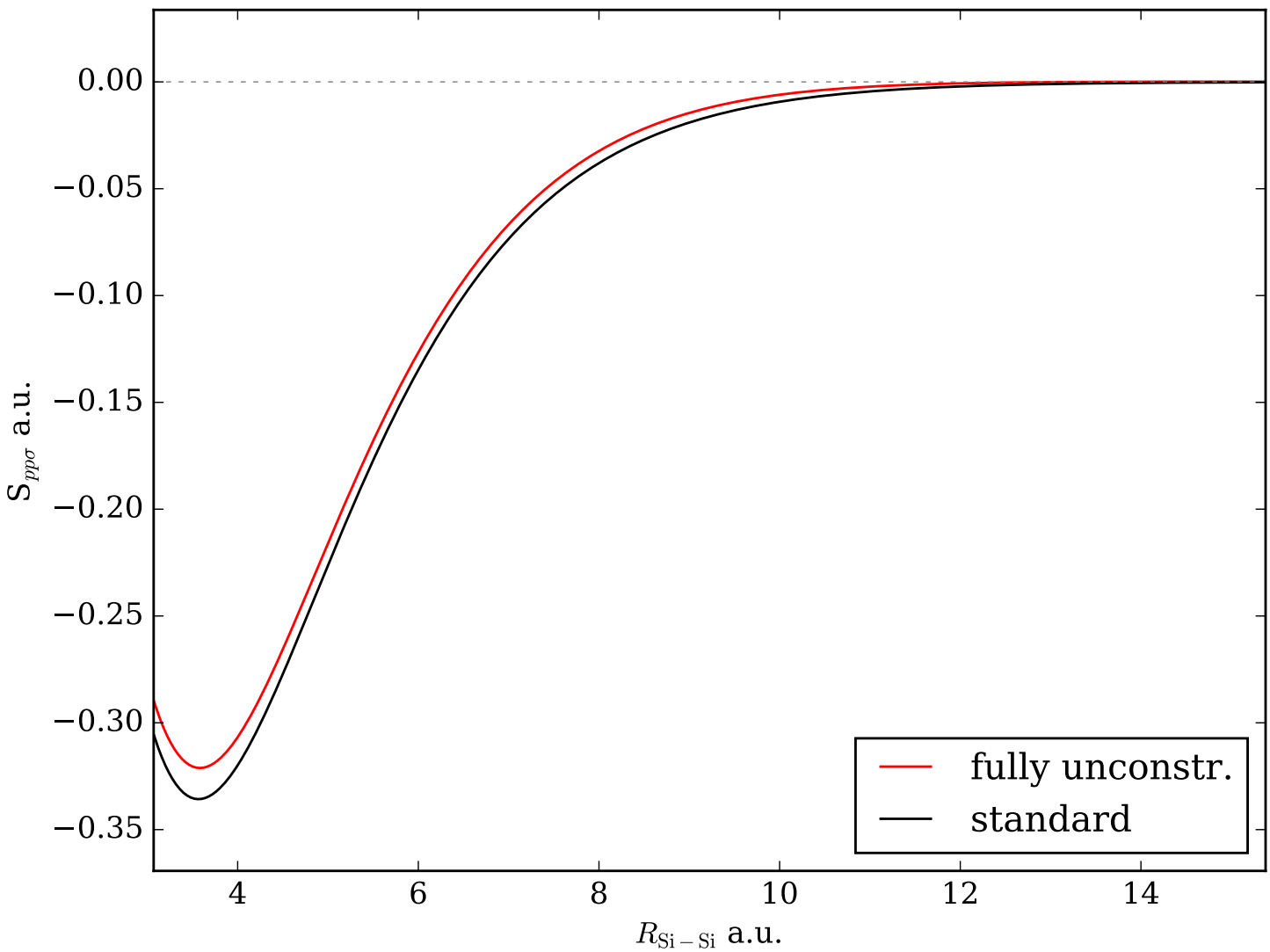
6
8
10
12
14
$R_{\mathrm{Si-Si}}$ a.u.
fully unconstr.
standard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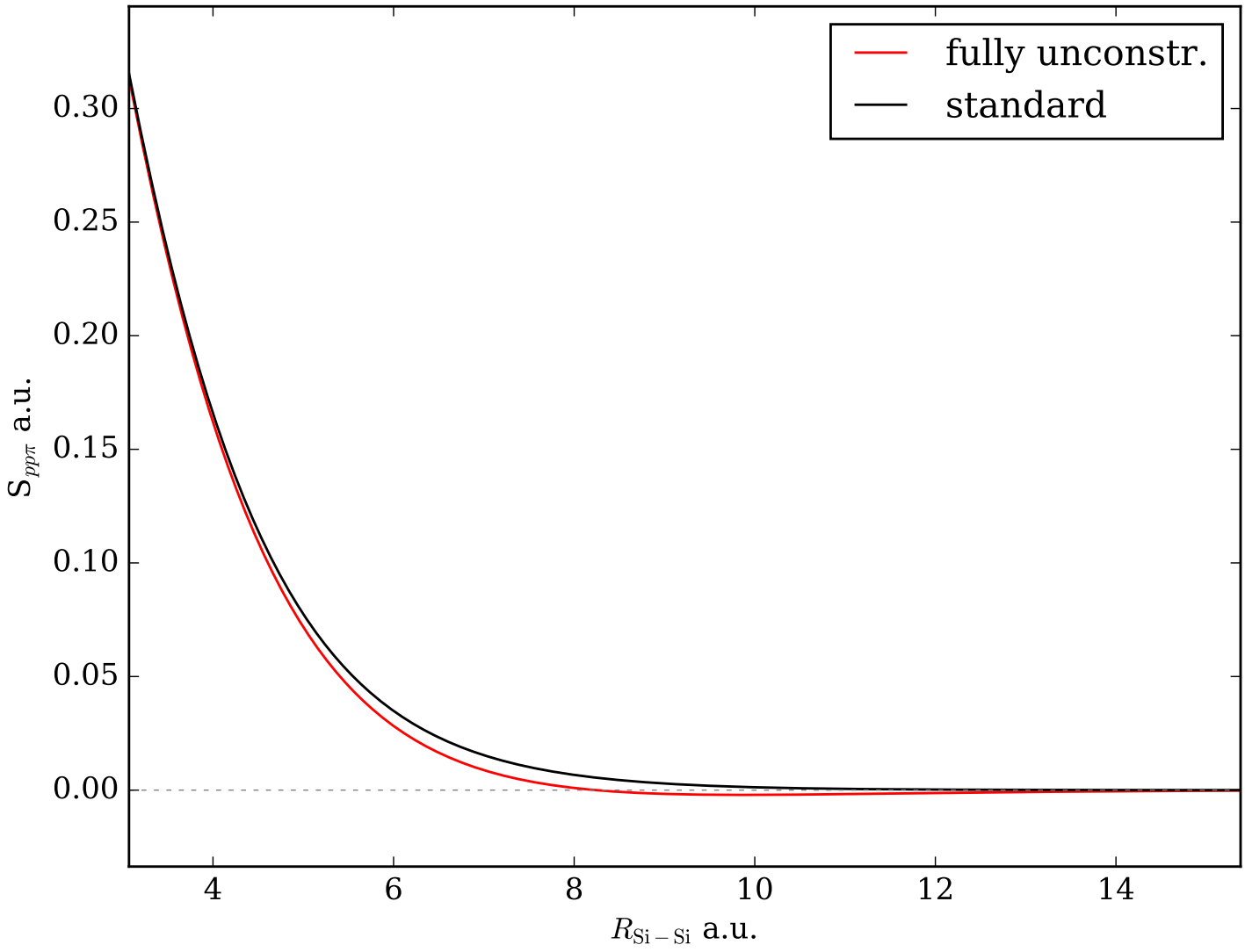
6
8
10
12
14
$R_{\mathrm{Si-Si}}$ a.u.
fully unconstr.
standard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standard
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0.15
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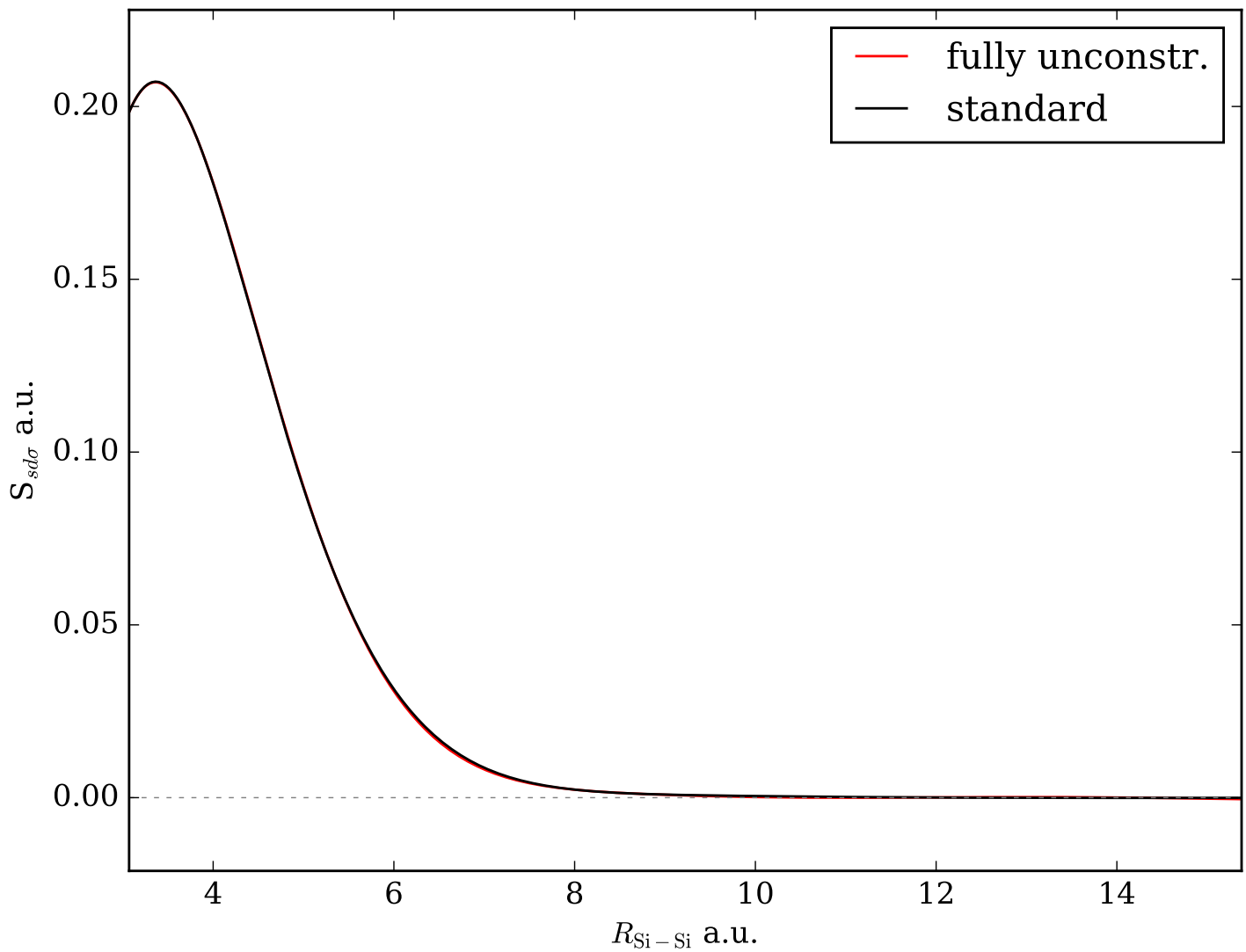
0.05
0.00
$S_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Si}}$ a.u.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standard
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0.05
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$S_{sd\sigma}$ a.u.
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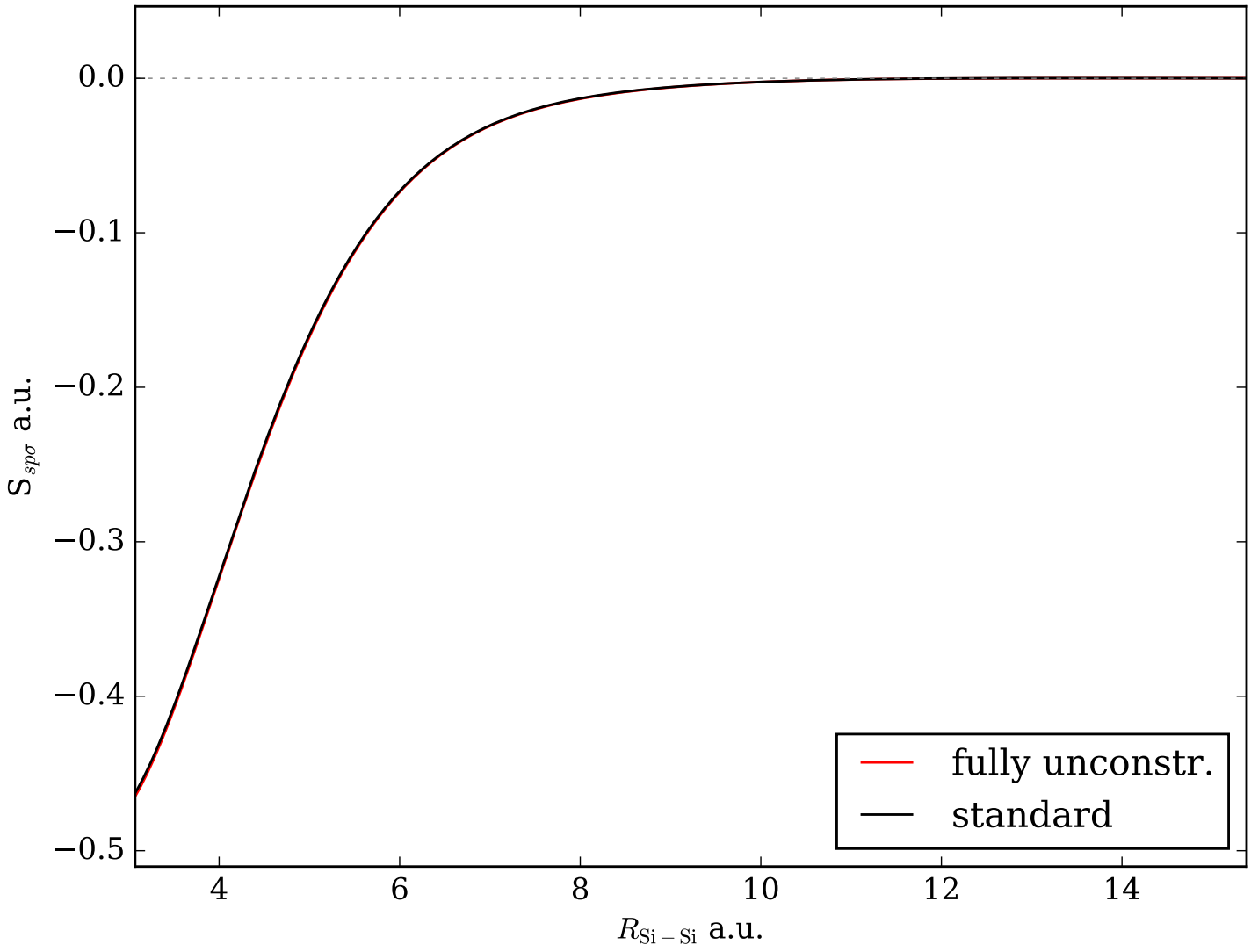
8
10
12
14
$R_{\mathrm{Si-Si}}$ a.u.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$S_{sp\sigma}$ a.u.
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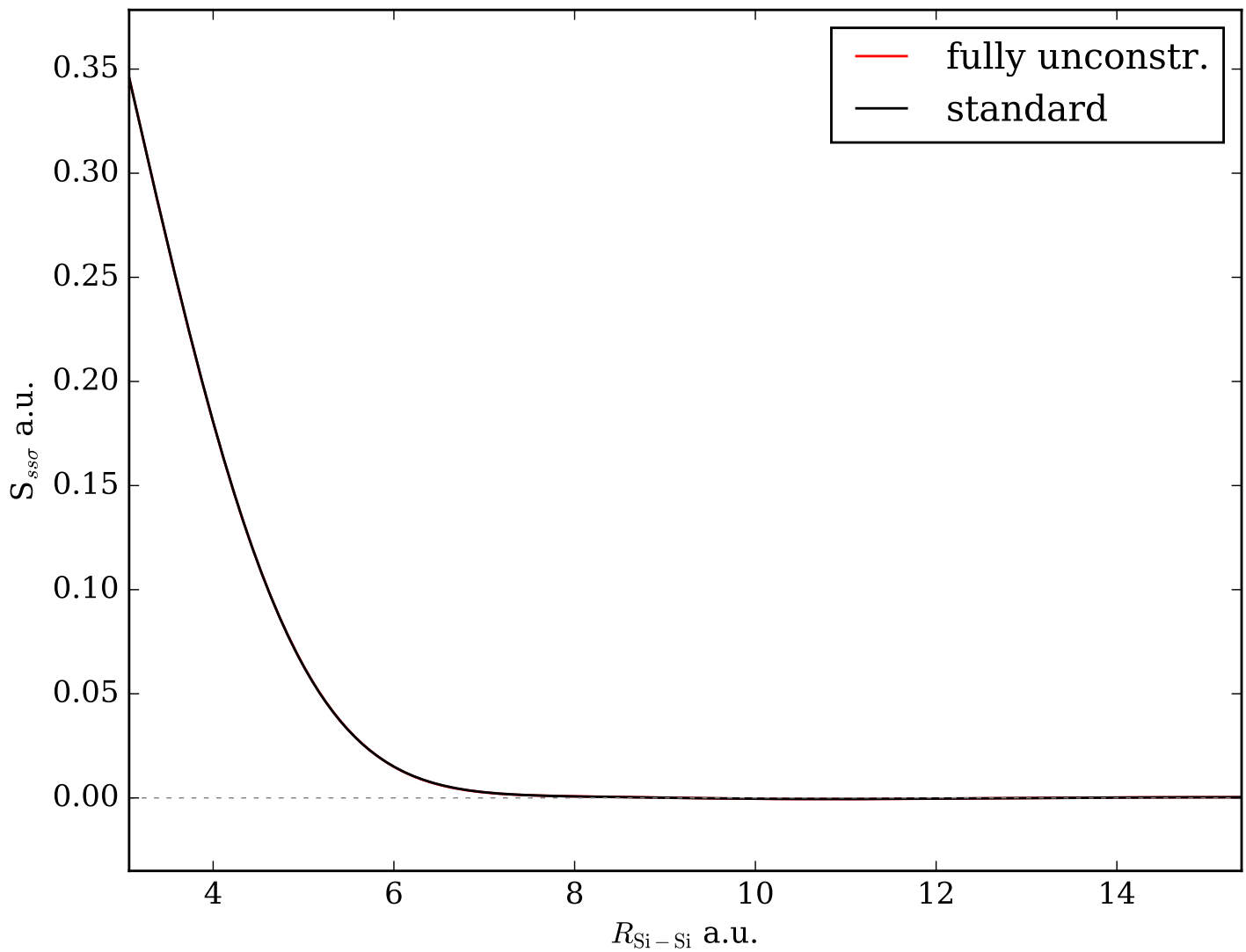
6
8
10
12
14
$R_{\mathrm{Si-Si}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
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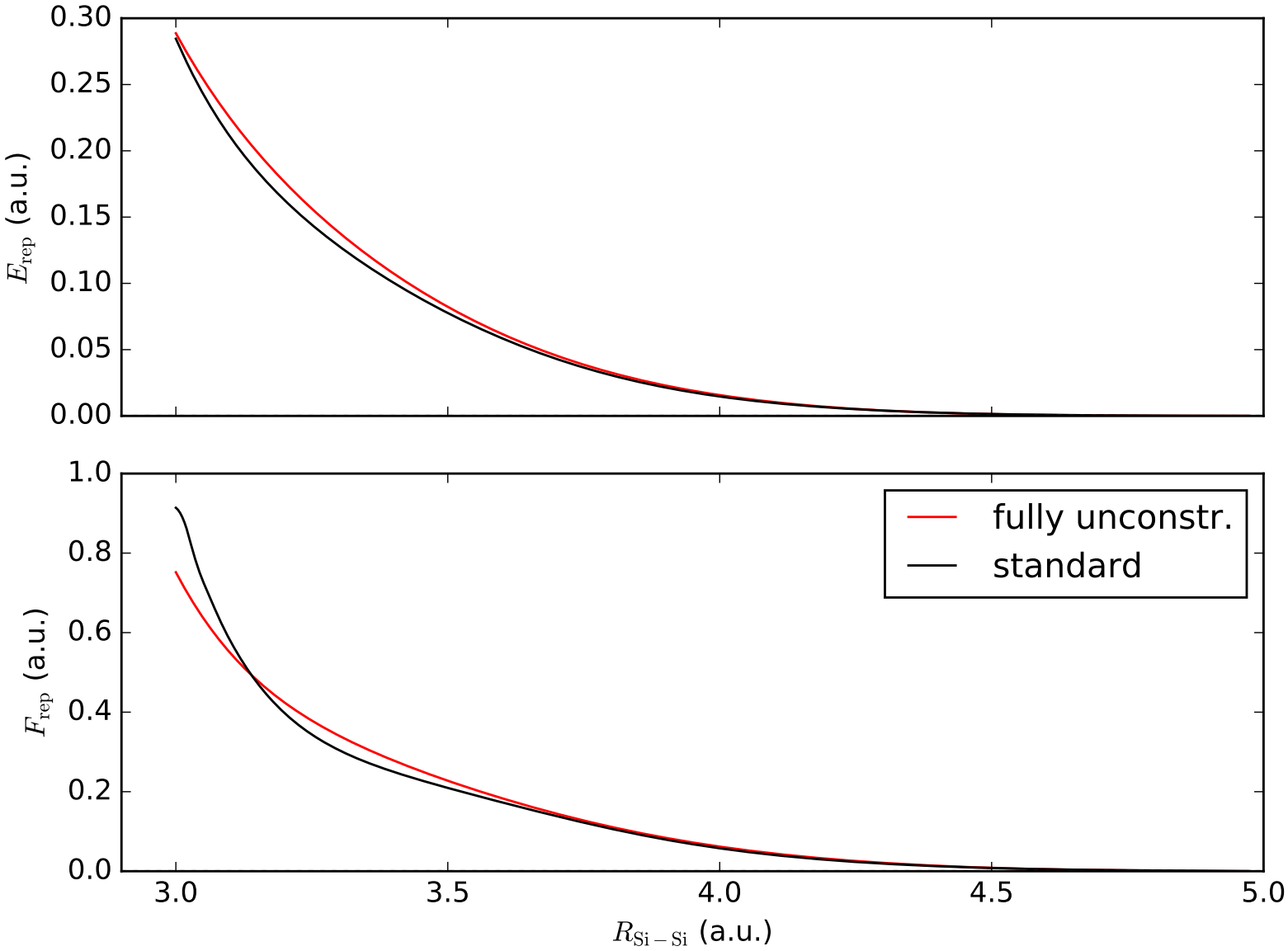
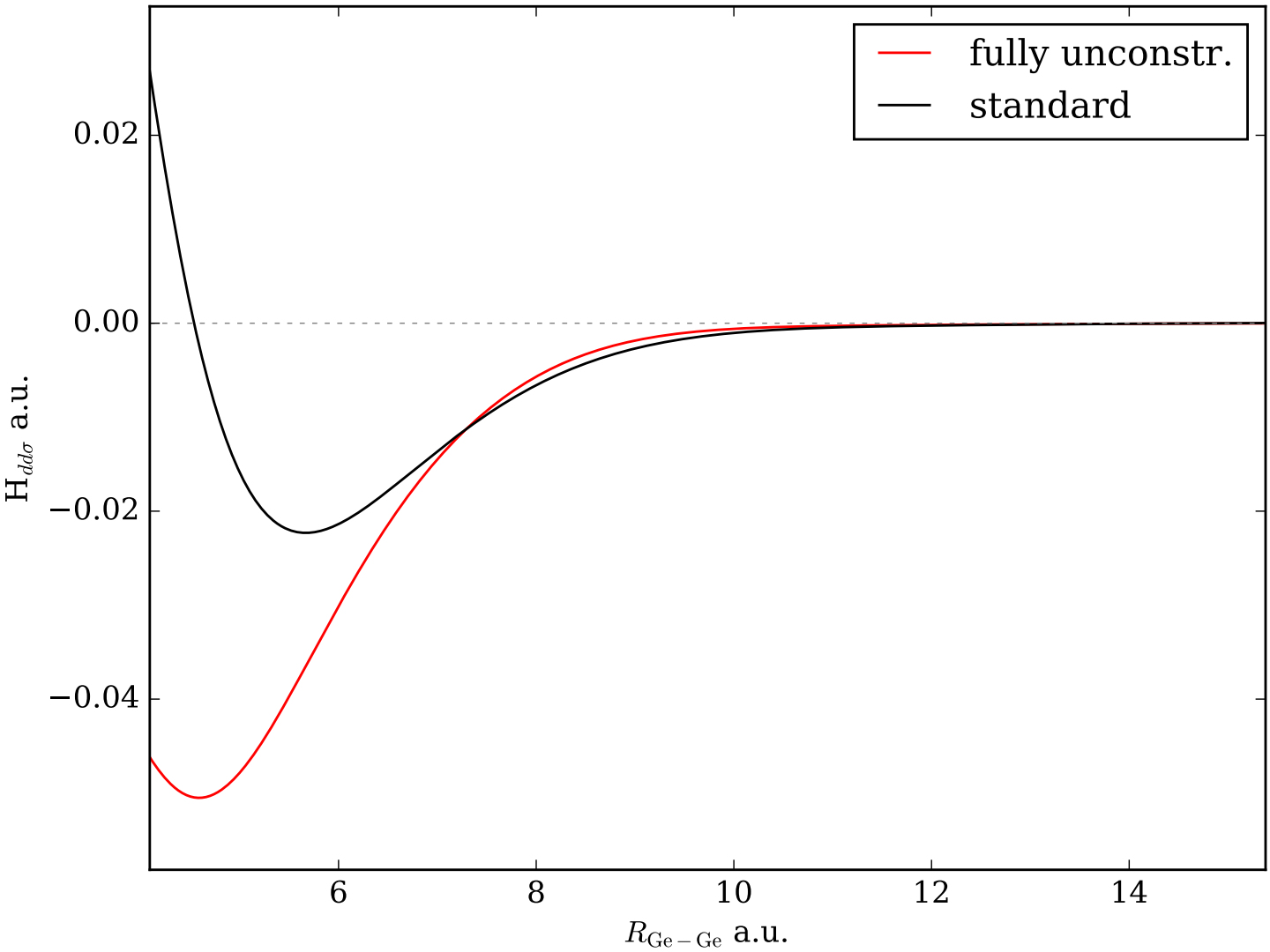
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$S_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Si}}$ a.u.

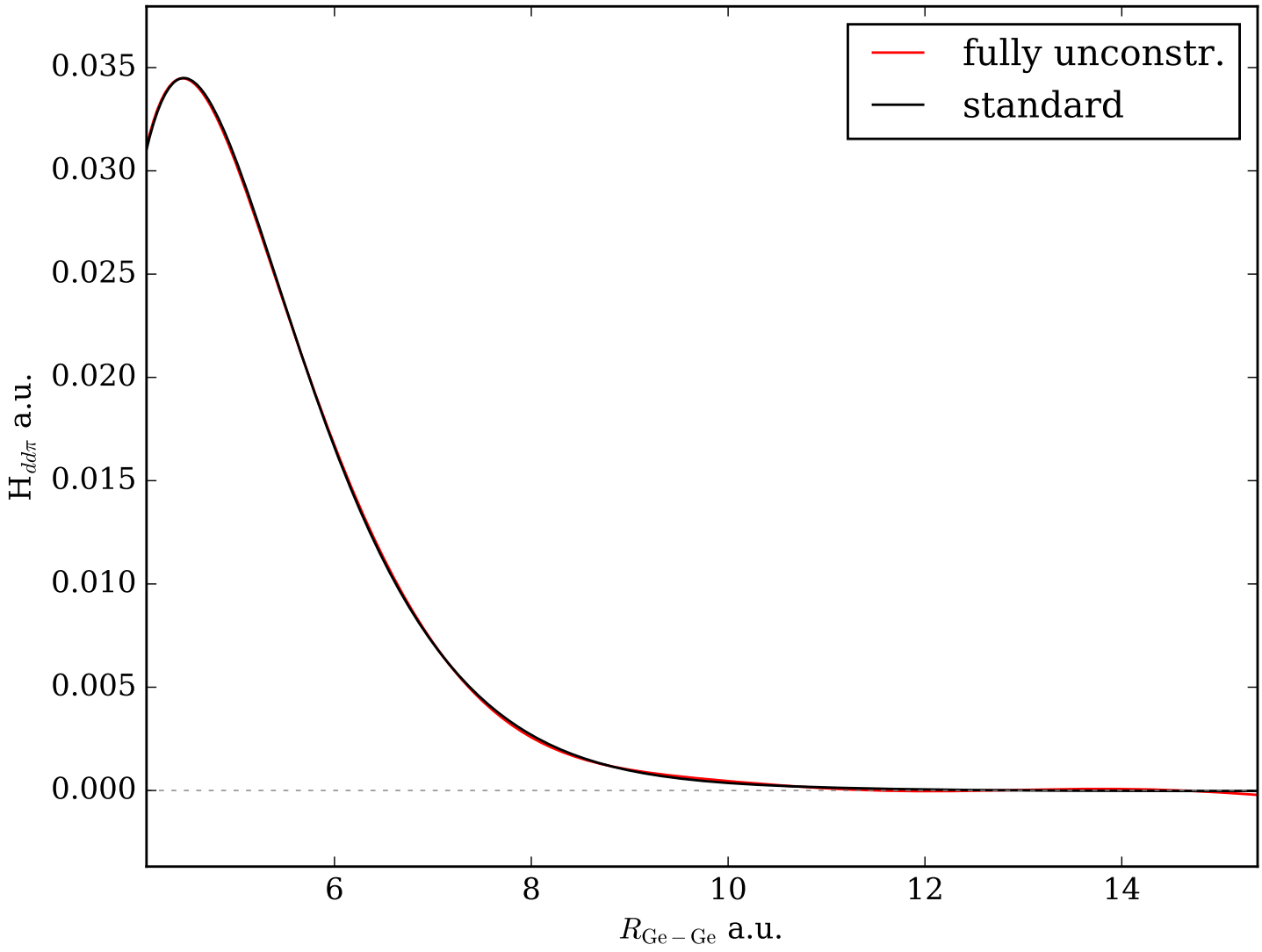
2.2 Repulsive

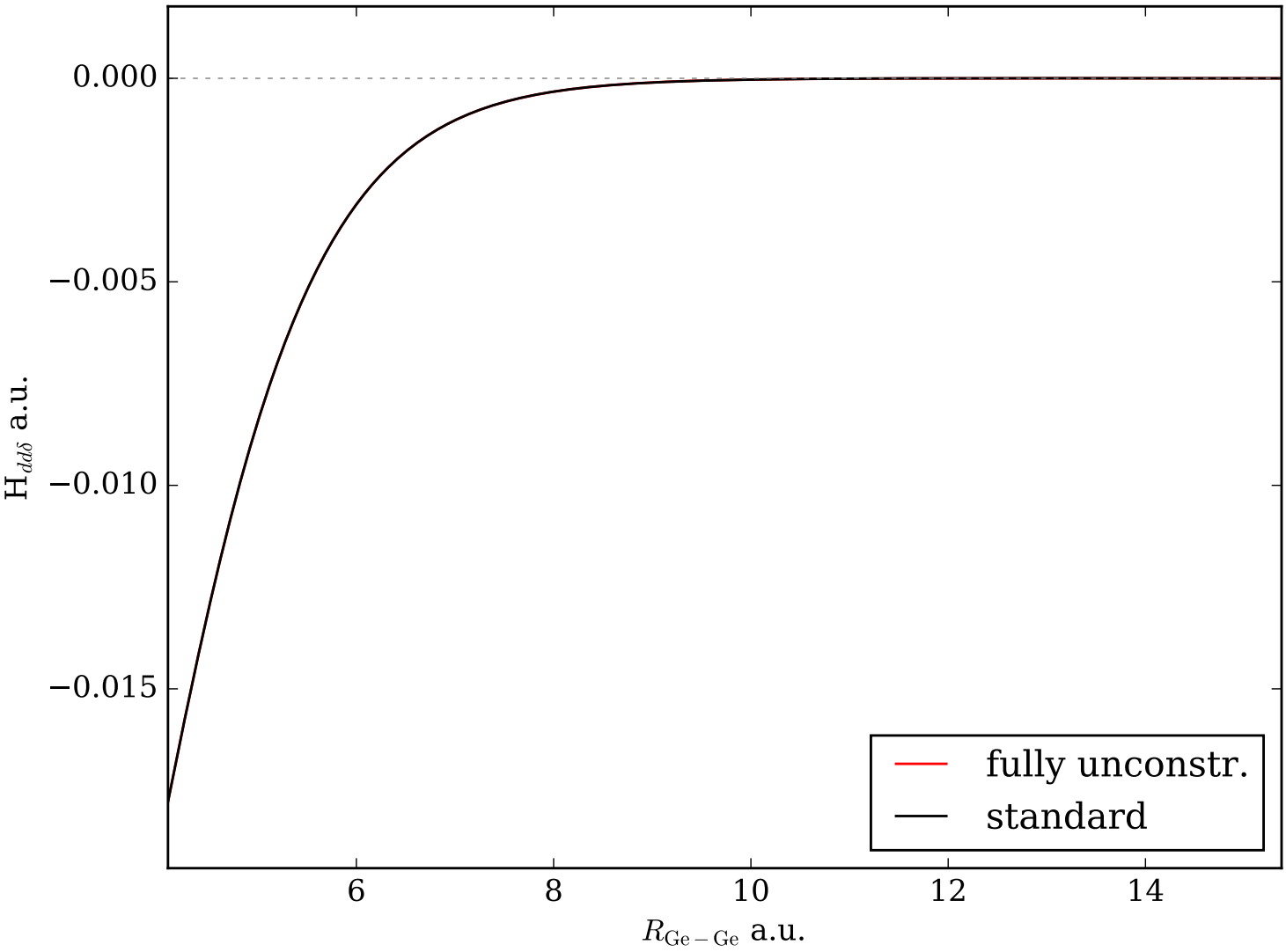


3 Ge-Ge

3.1 Electronic




fully unconstr.
standard
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
$H_{dd\pi}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.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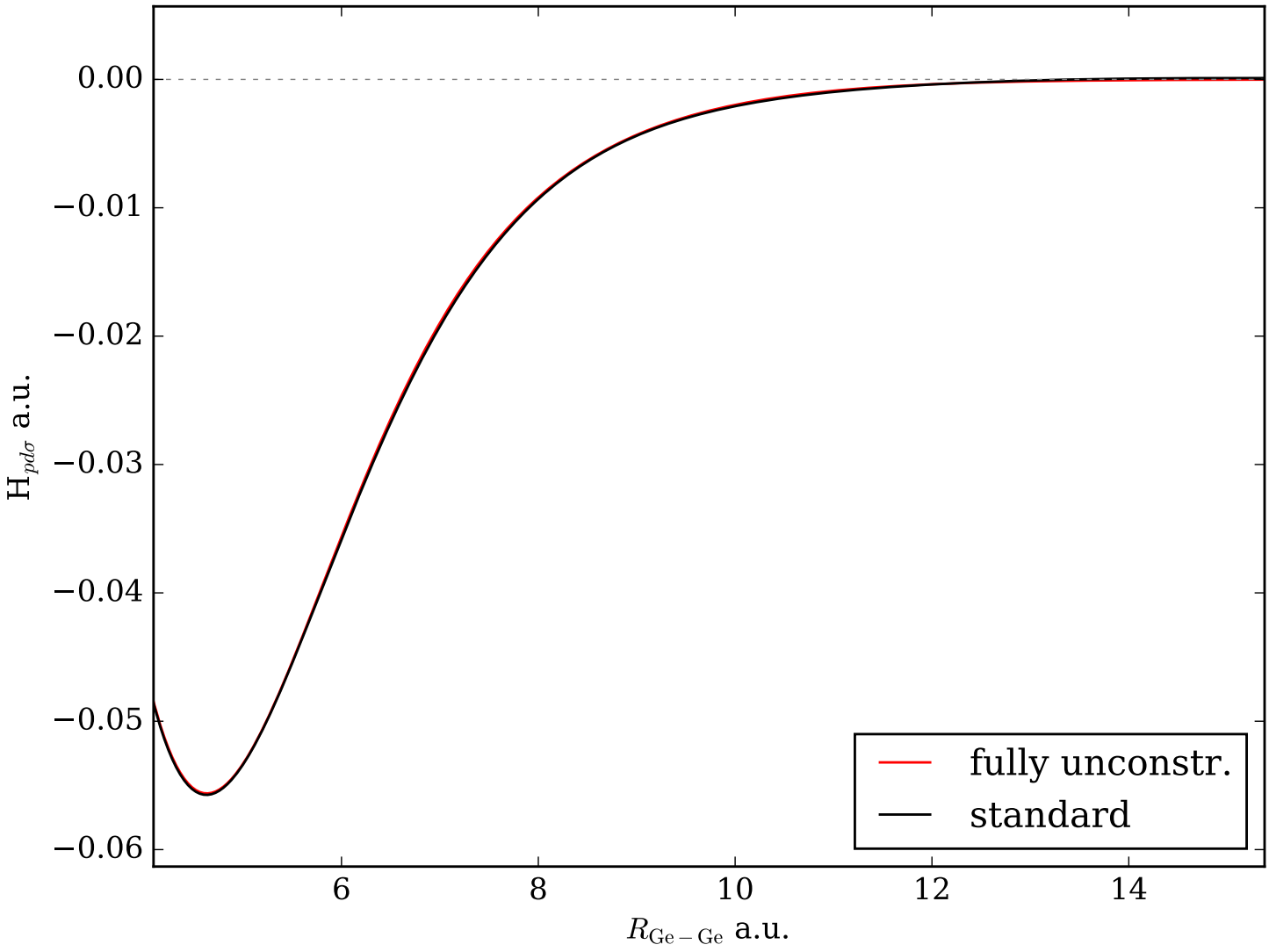
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.
fully unconstr.
standard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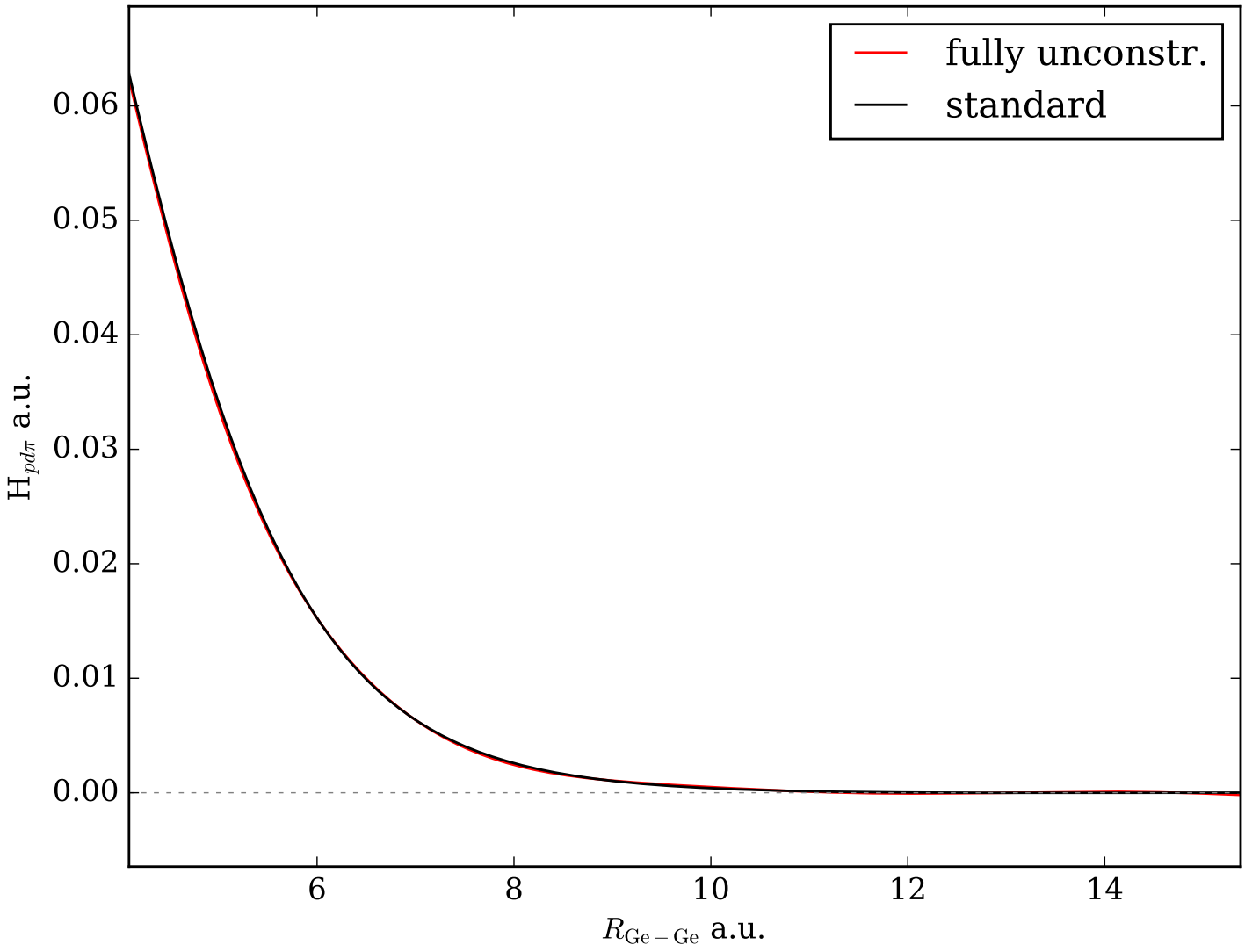
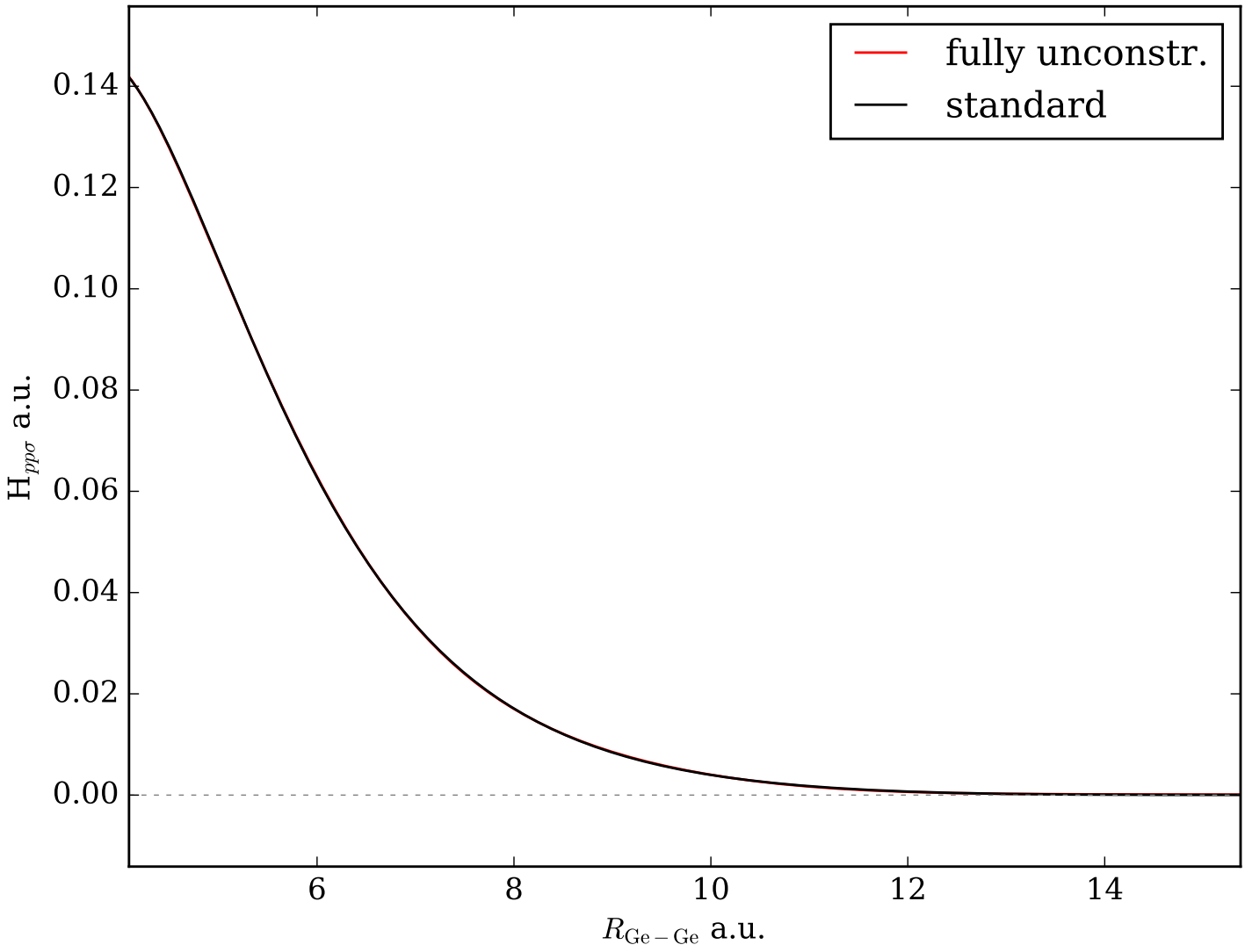
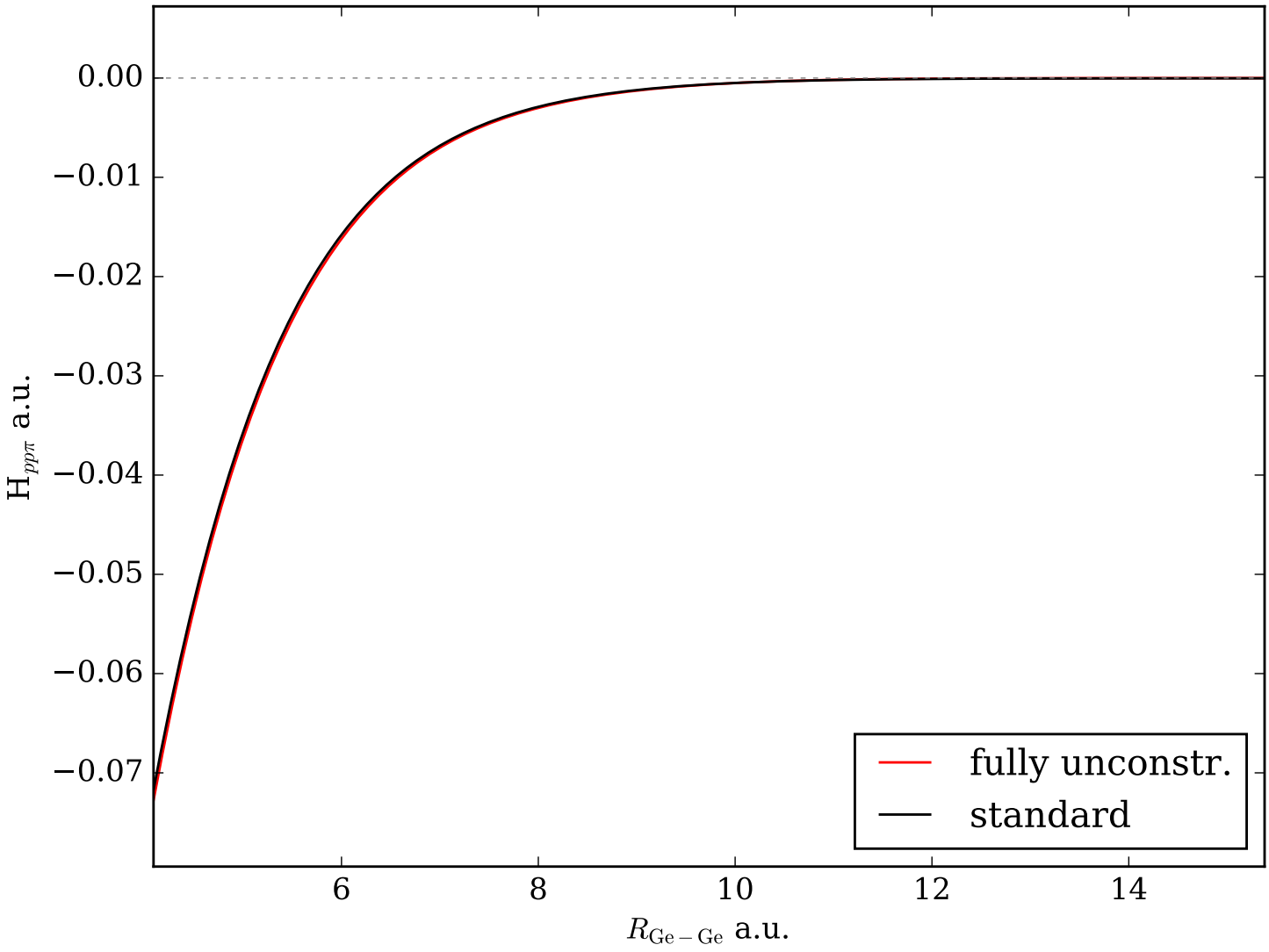
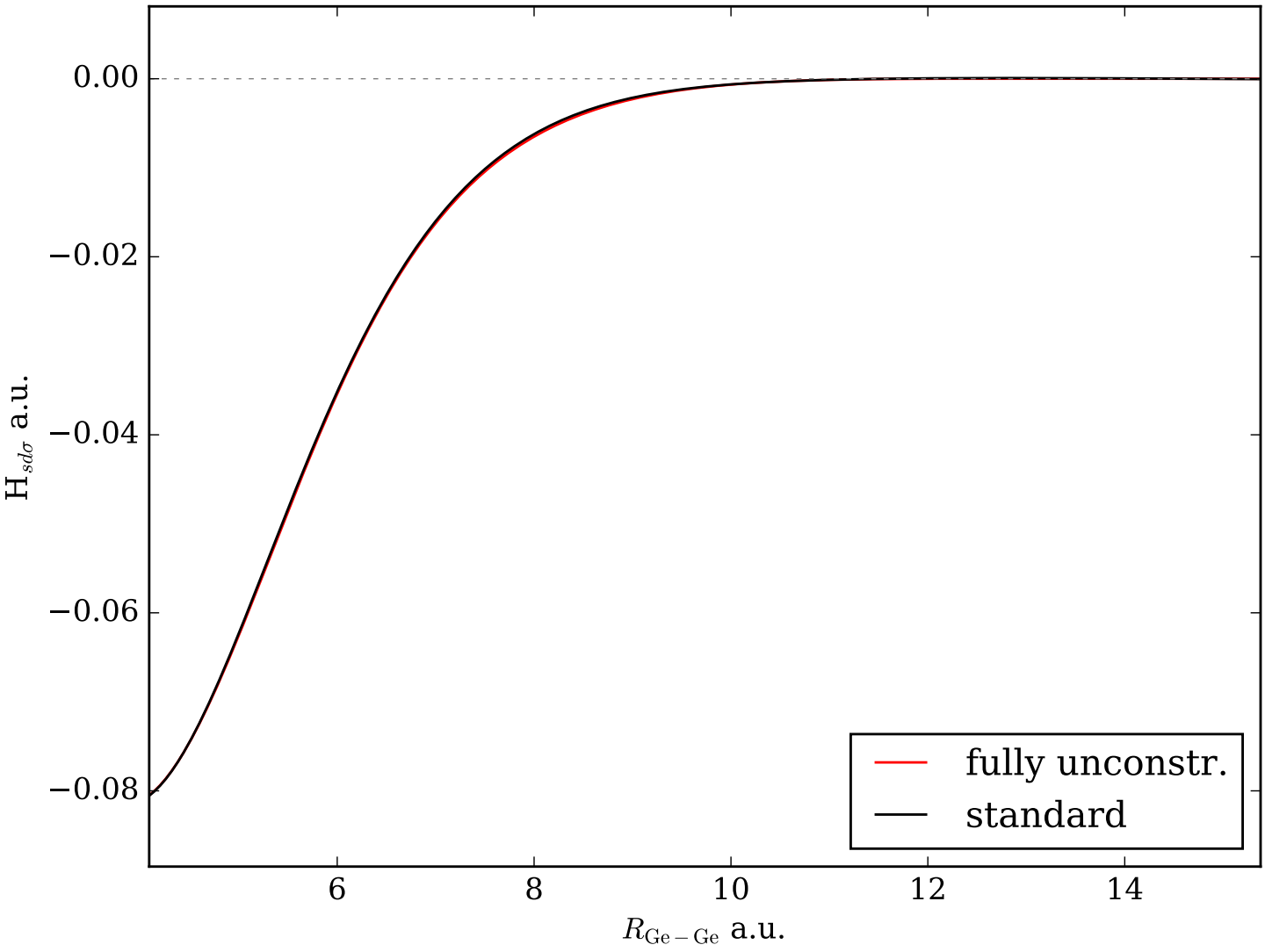
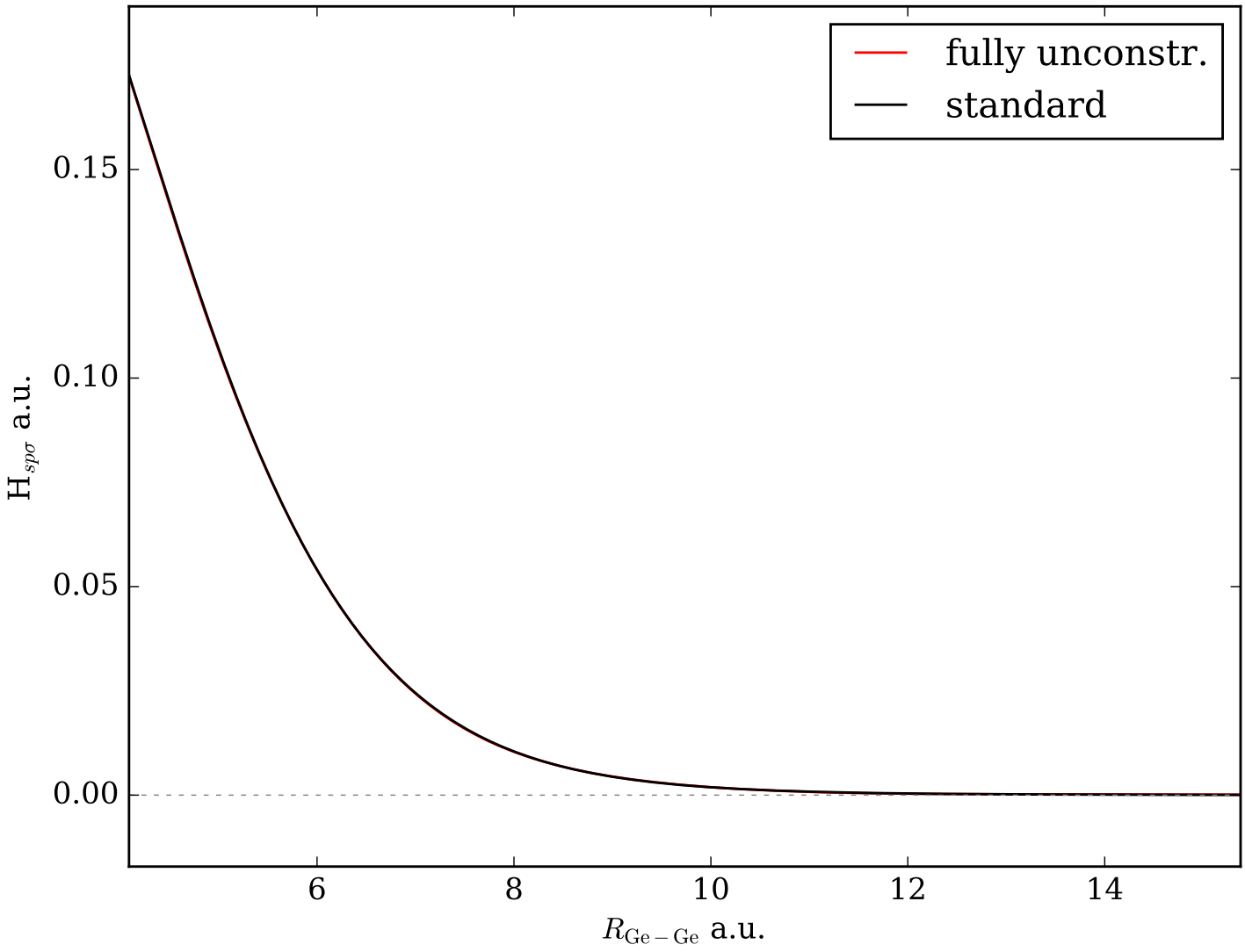
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.
fully unconstr.
standard

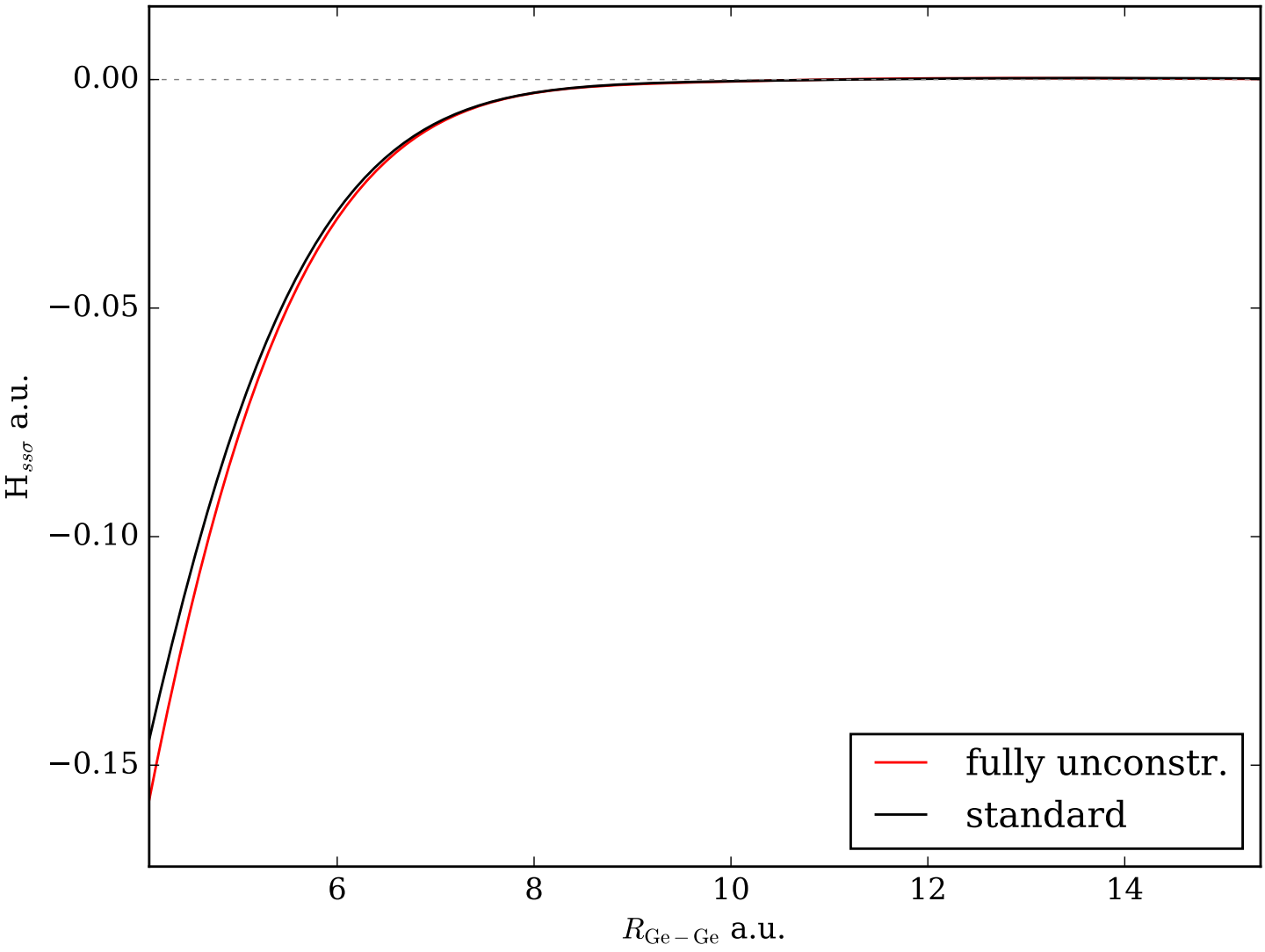

fully unconstr.
standard
0.06
0.05
0.04
0.03
0.02
0.01
0.00
$H_{pd\pi}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.

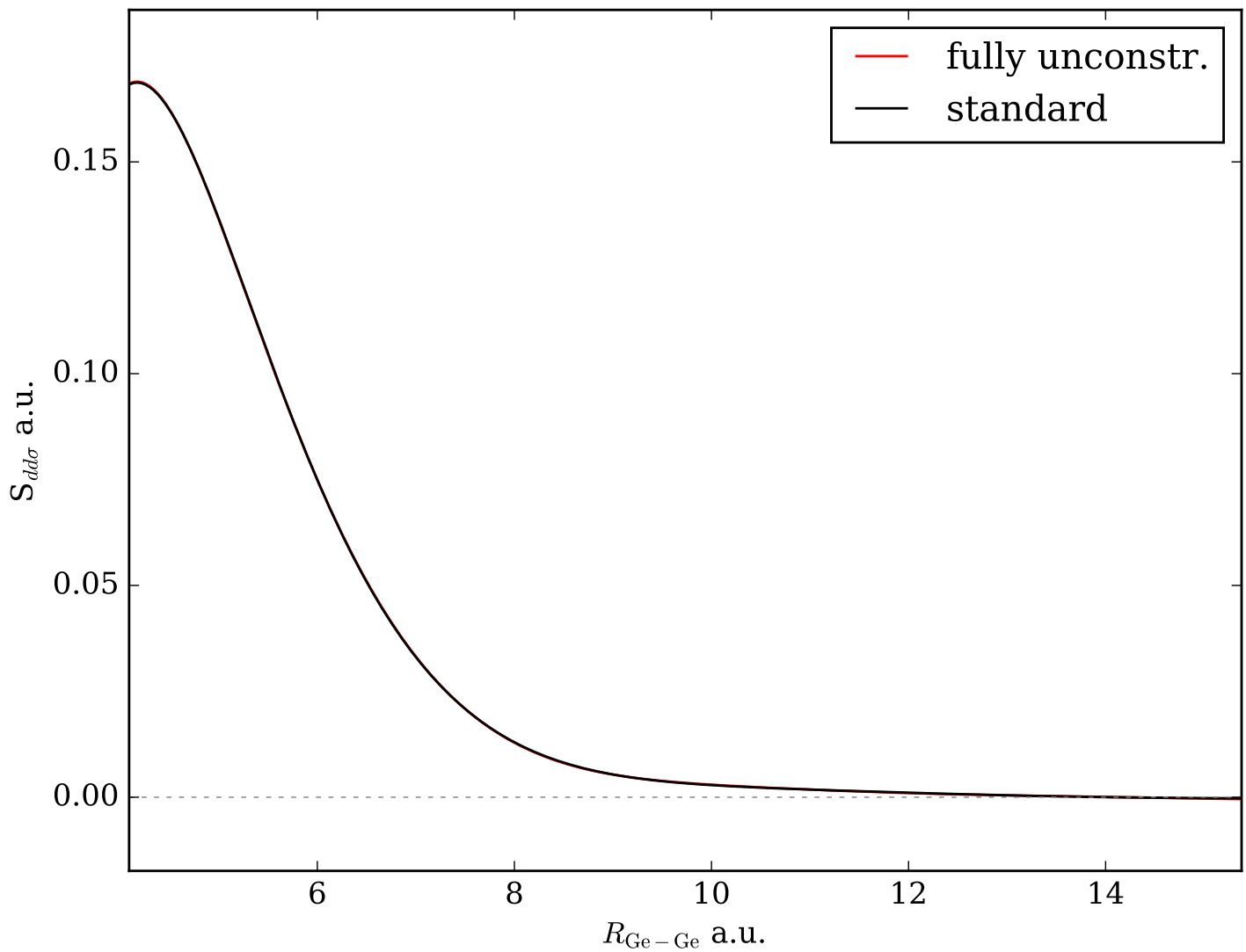

fully unconstr.
standard
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
$H_{pp\sigma}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.

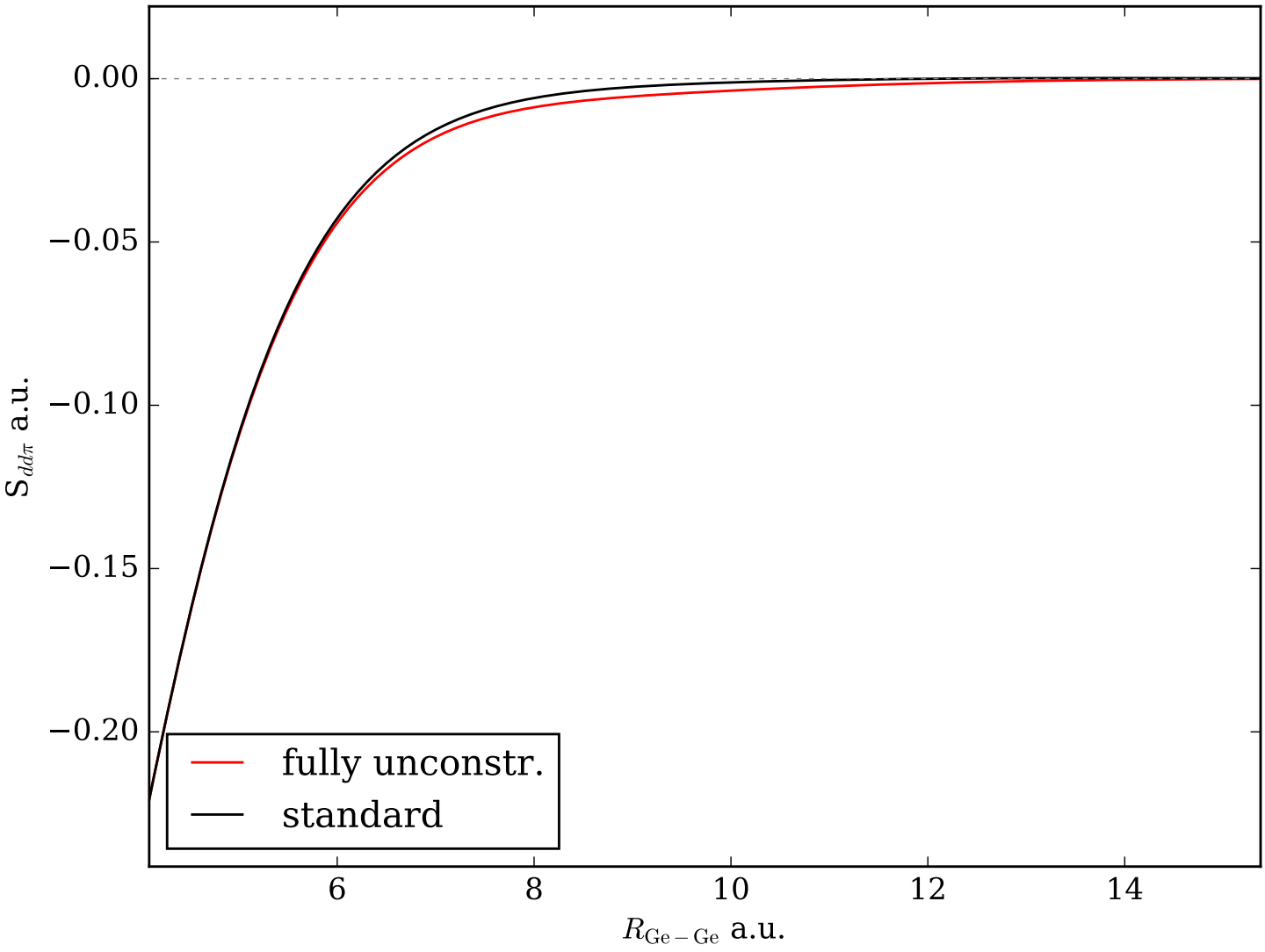

0.00
−0.01
−0.02
−0.03
−0.04
−0.05
−0.06
−0.07
$H_{pp\pi}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.
fully unconstr.
standard

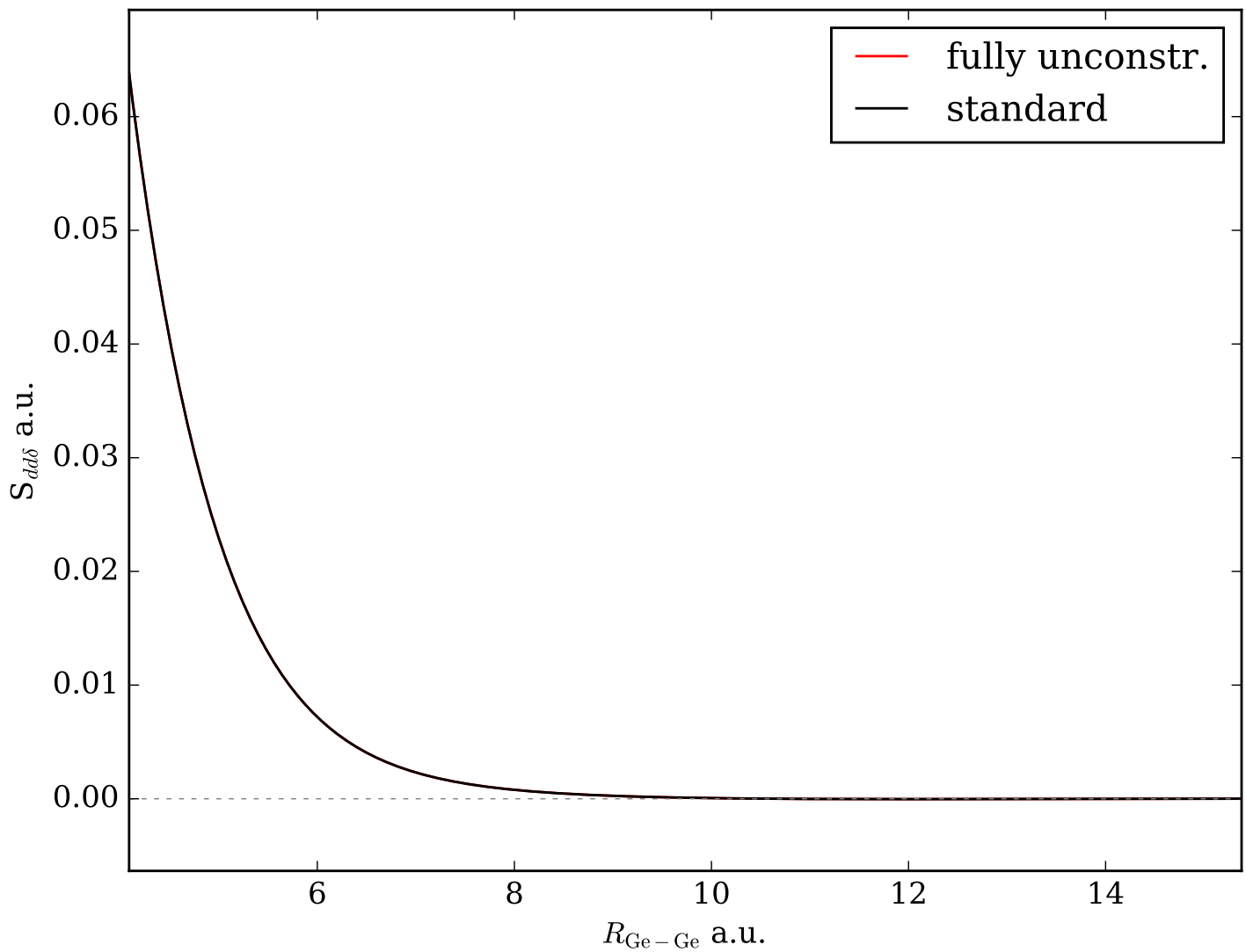

0.00
−0.02
−0.04
−0.06
−0.08
$H_{sd\sigma}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.
fully unconstr.
standard

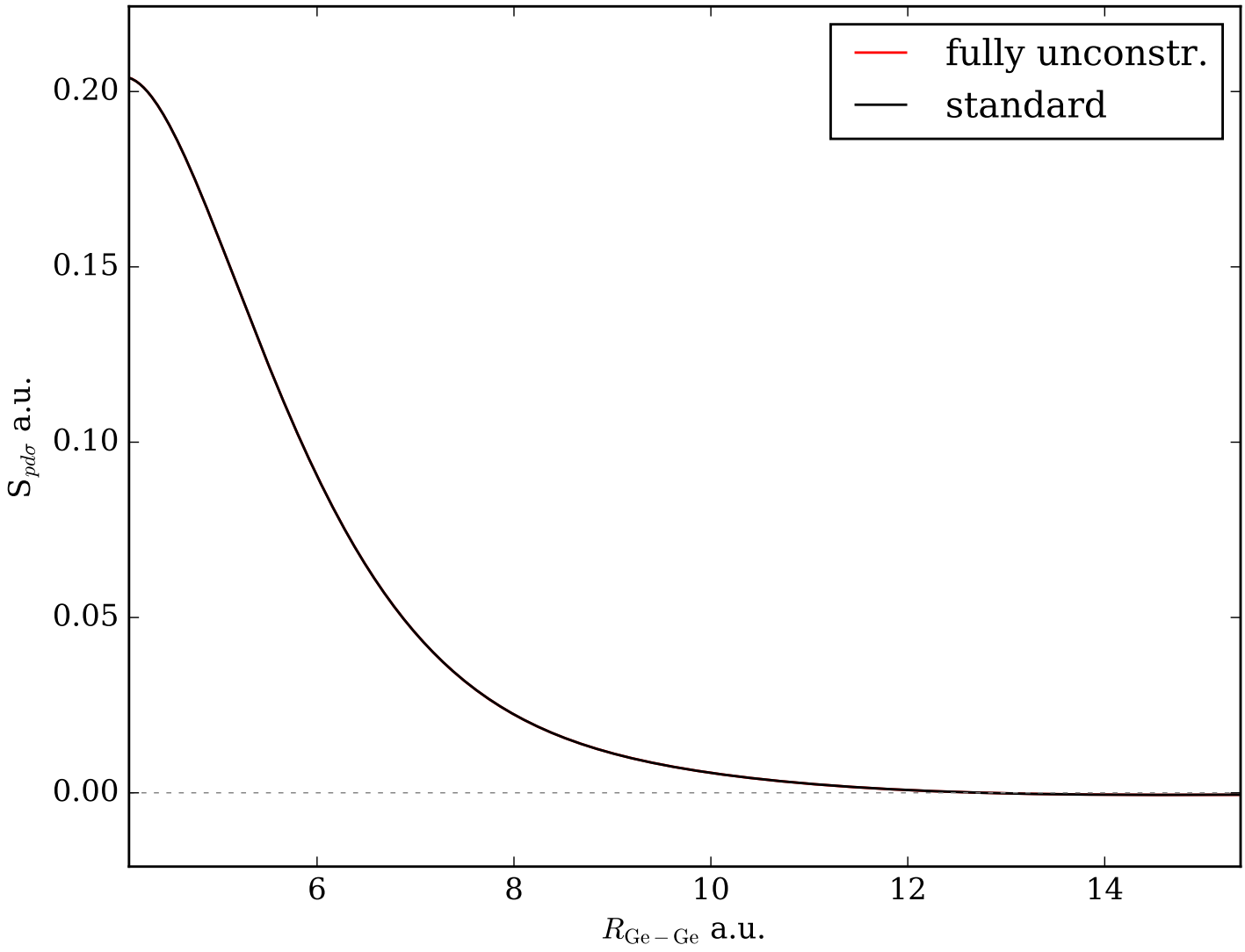

fully unconstr.
standard
0.15
0.10
0.05
0.00
$H_{sp\sigma}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.

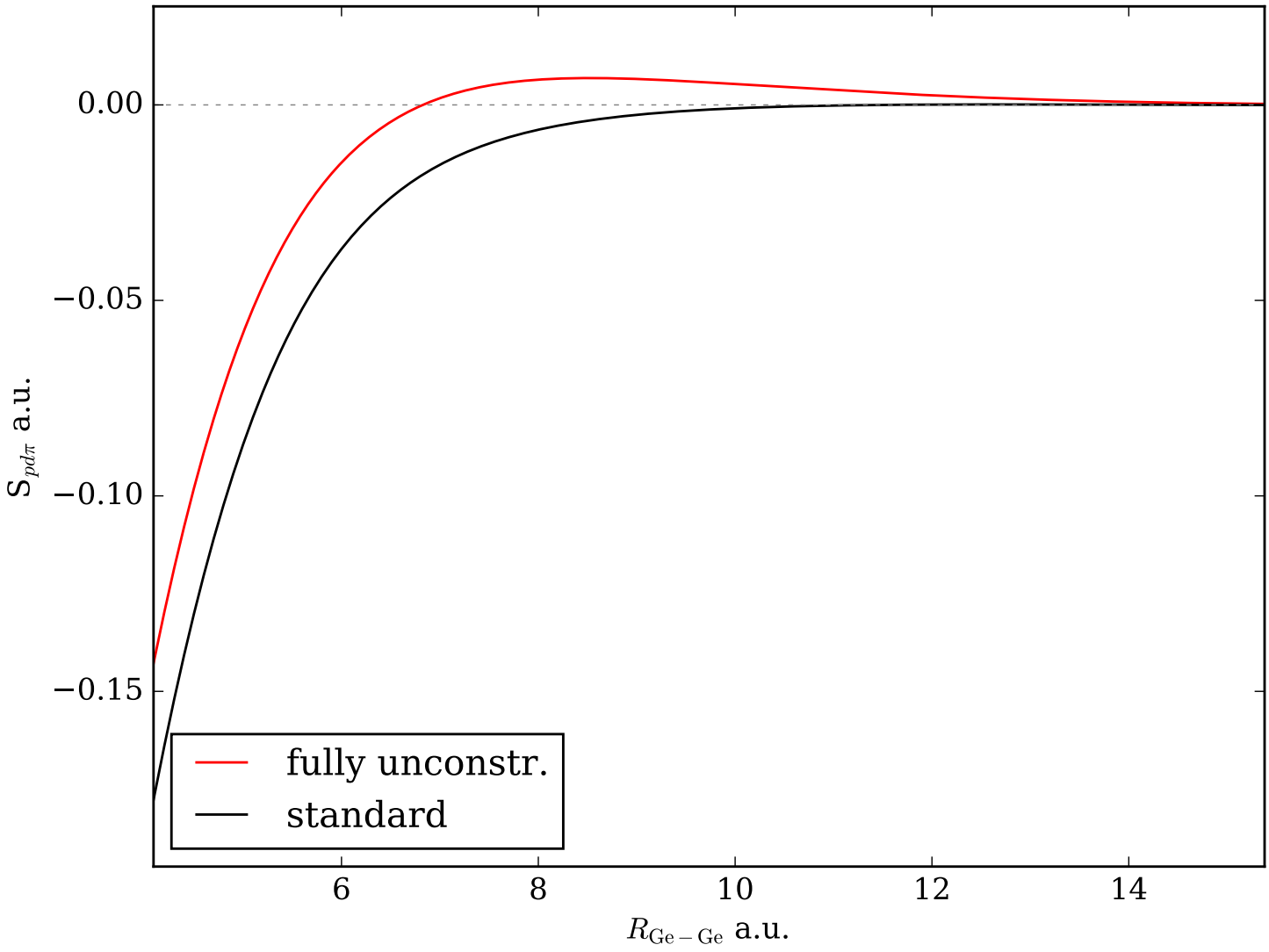

0.00
−0.05
−0.10
−0.15
$H_{ss\sigma}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.
fully unconstr.
standard

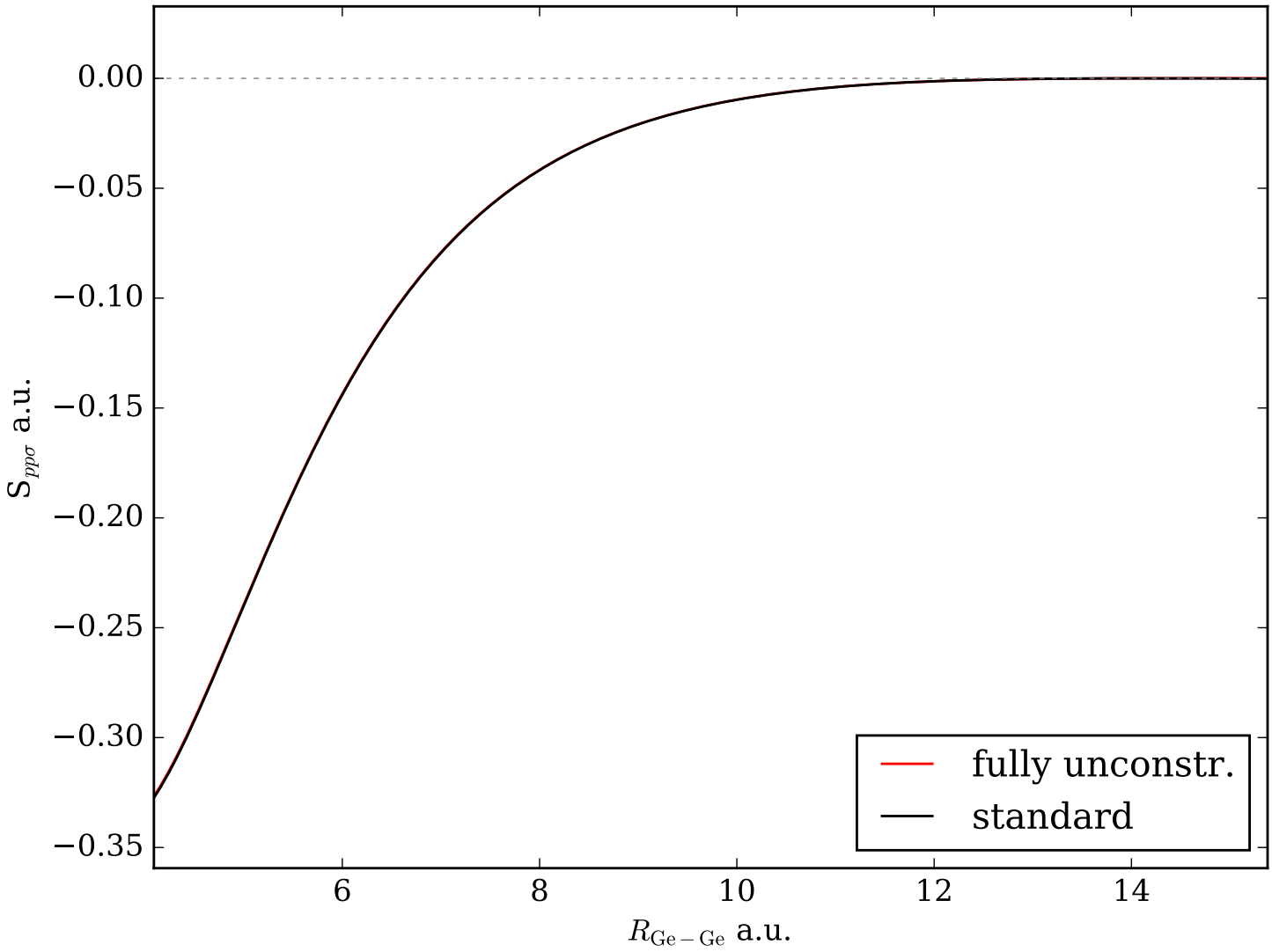

fully unconstr.
standard
0.15
0.10
0.05
0.00
$S_{dd\sigma}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.

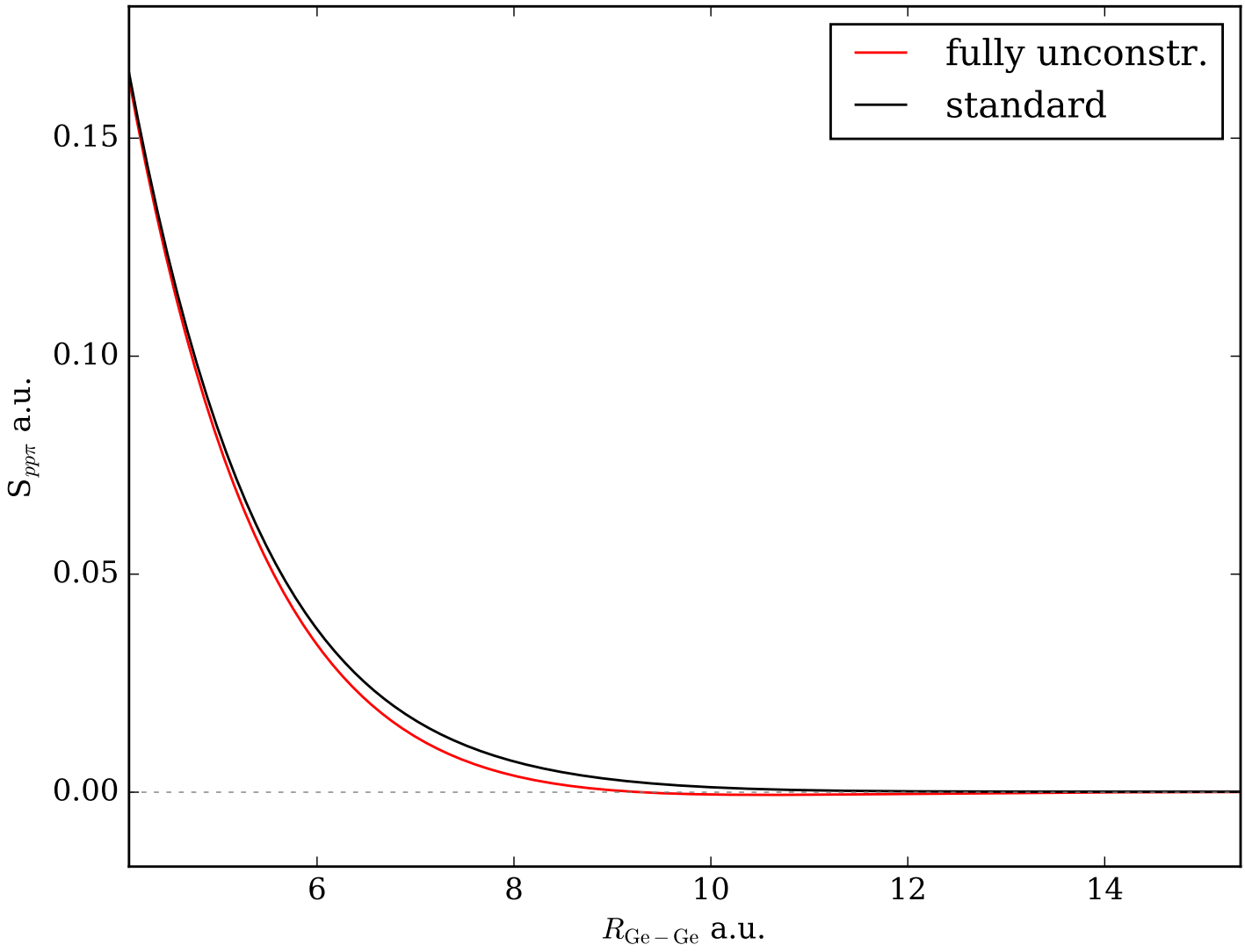

0.00
−0.05
−0.10
−0.15
−0.20
$S_{dd\pi}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.
fully unconstr.
standard

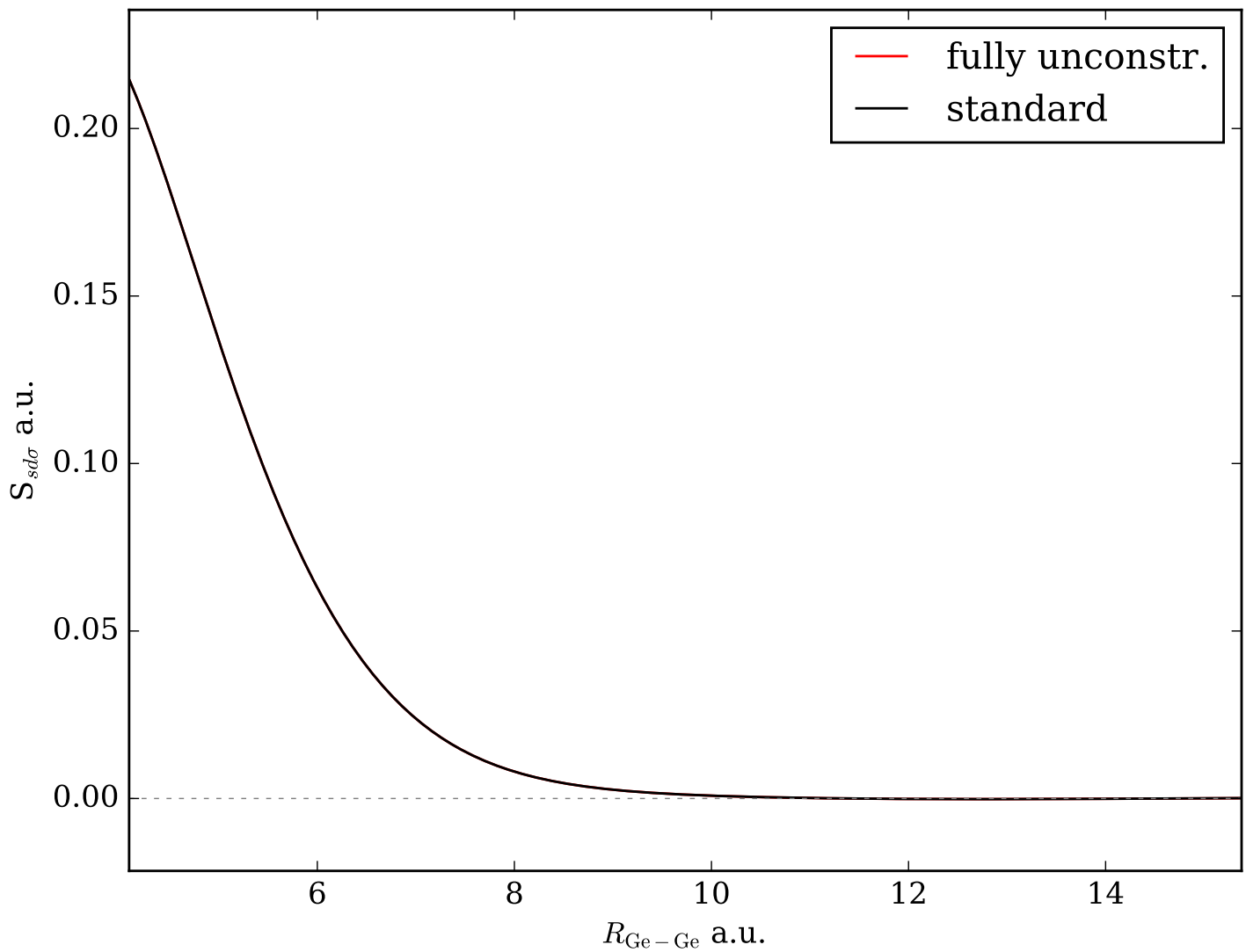

fully unconstr.
standard
0.06
0.05
0.04
0.03
0.02
0.01
0.00
$S_{dd\delta}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.

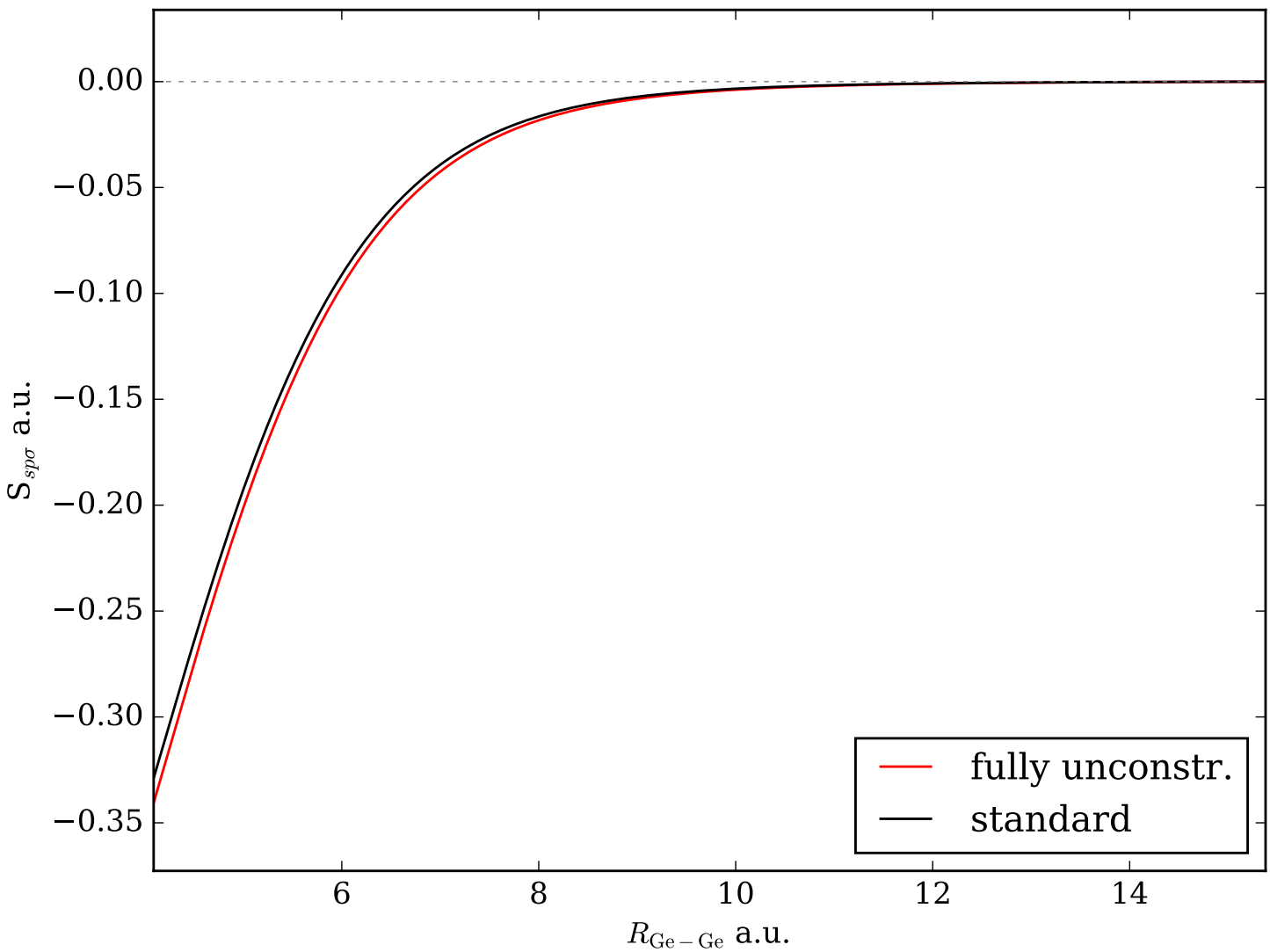

fully unconstr.
standard
0.20
0.15
0.10
0.05
0.00
$S_{pd\sigma}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.

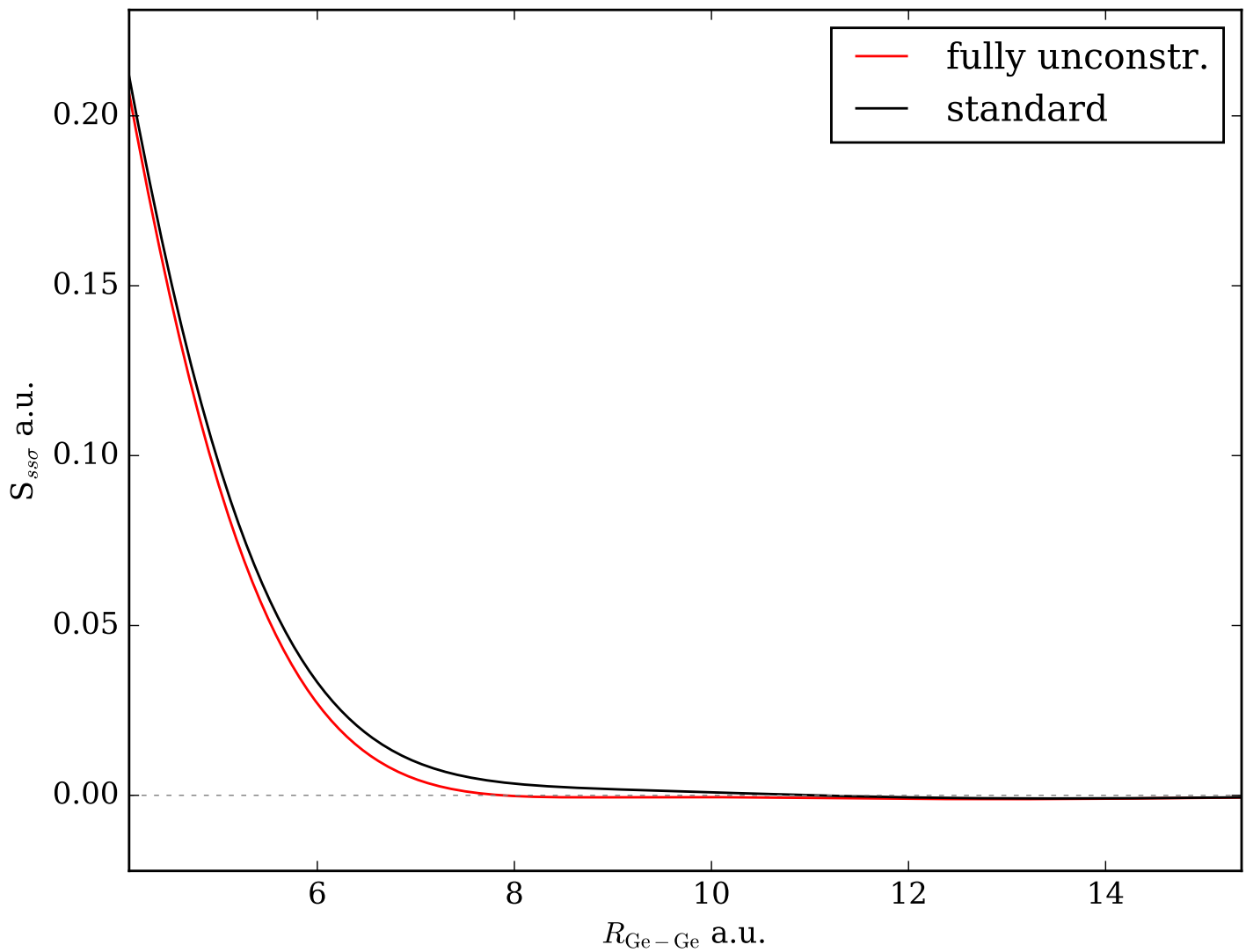

0.00
−0.05
−0.10
−0.15
$S_{pd\pi}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.
fully unconstr.
standard


0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
−0.35
$S_{pp\sigma}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.
fully unconstr.
standard

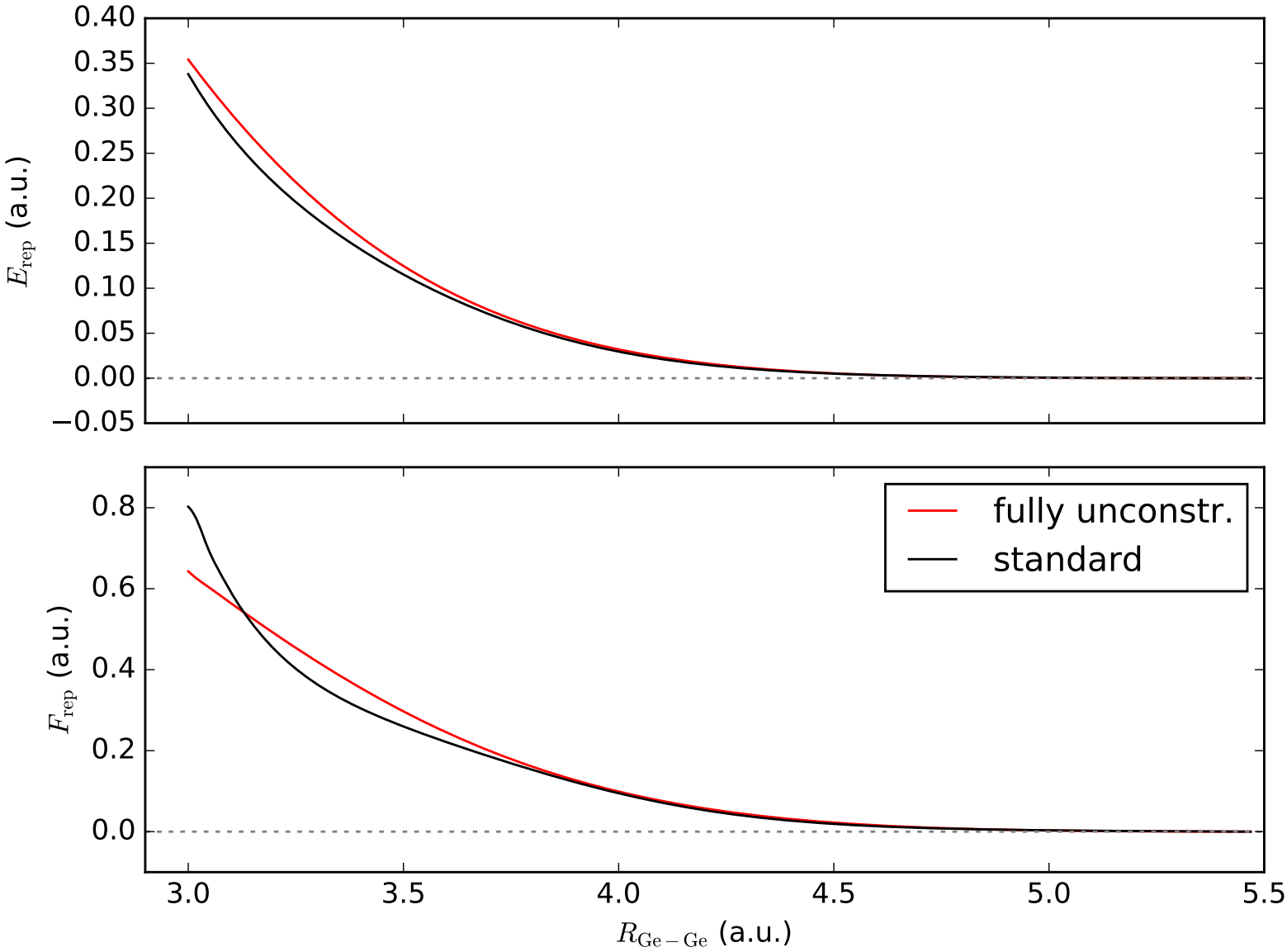

fully unconstr.
standard
0.15
0.10
0.05
0.00
$S_{pp\pi}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.


fully unconstr.
standard
0.20
0.15
0.10
0.05
0.00
$S_{sd\sigma}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.


0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
−0.35
$S_{sp\sigma}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.
fully unconstr.
standard

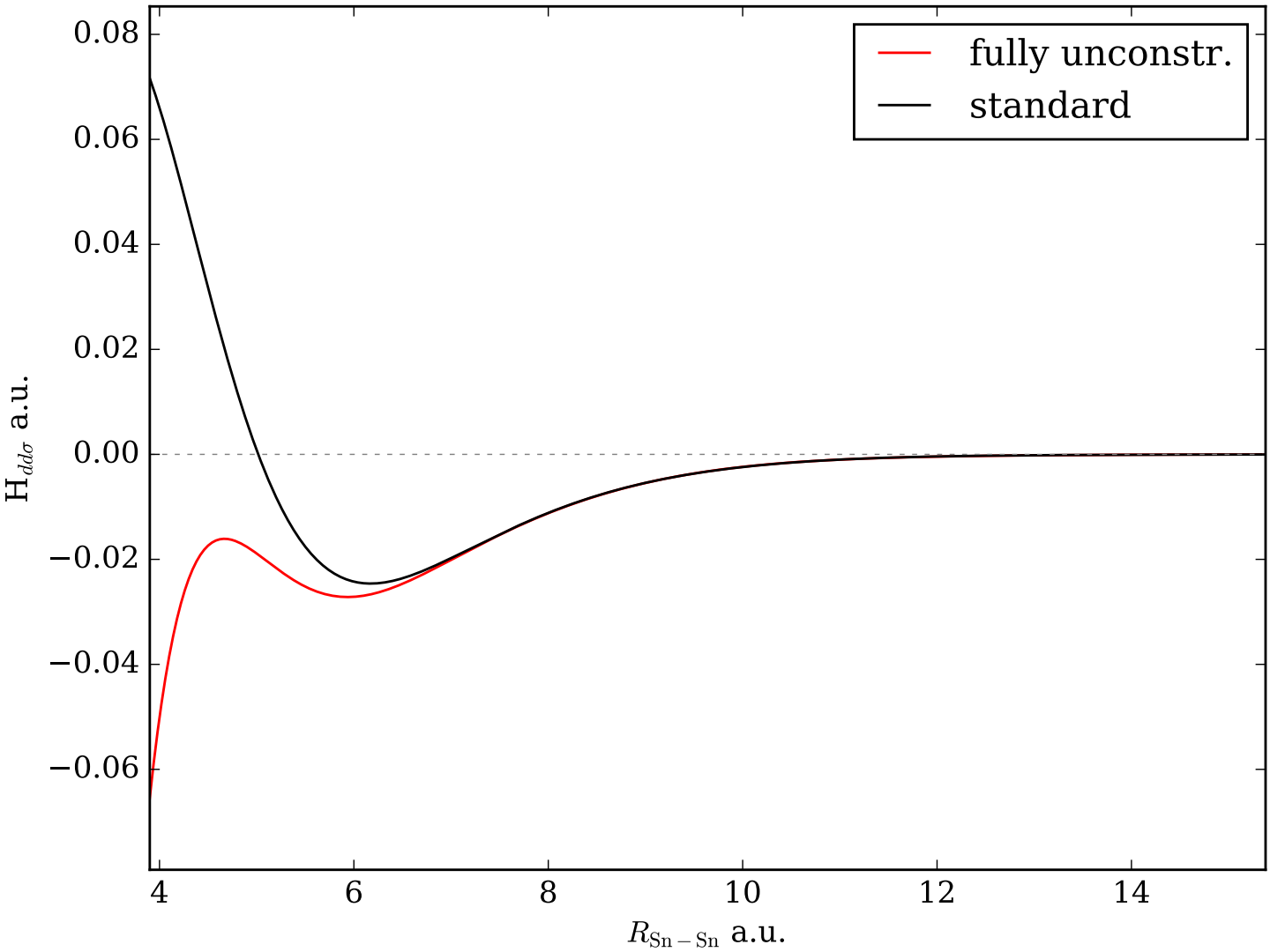

fully unconstr.
standard
0.20
0.15
0.10
0.05
0.00
$S_{ss\sigma}$ a.u.
6
8
10
12
14
$R_{\mathrm{Ge-Ge}}$ a.u.

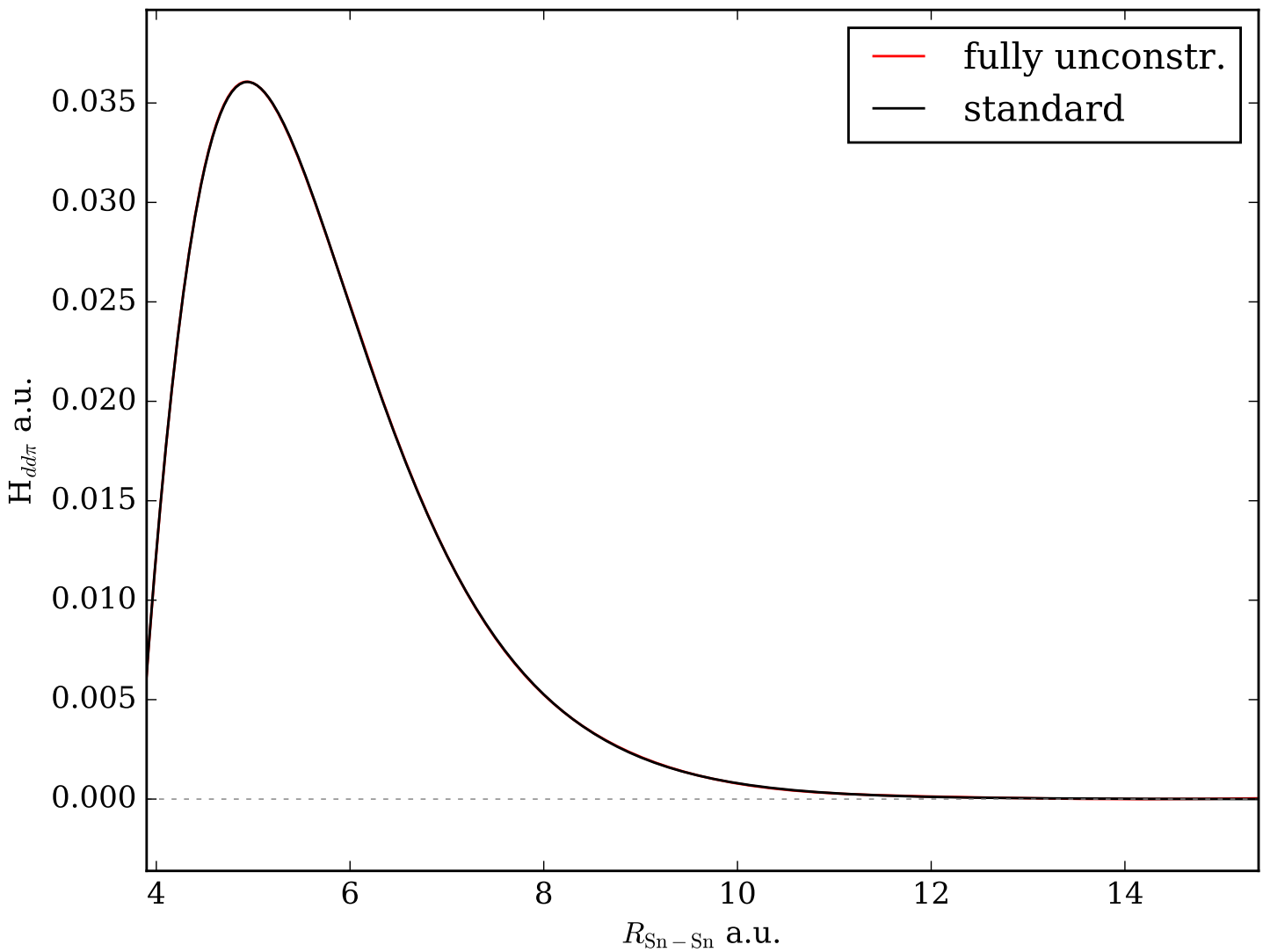
3.2 Repulsive

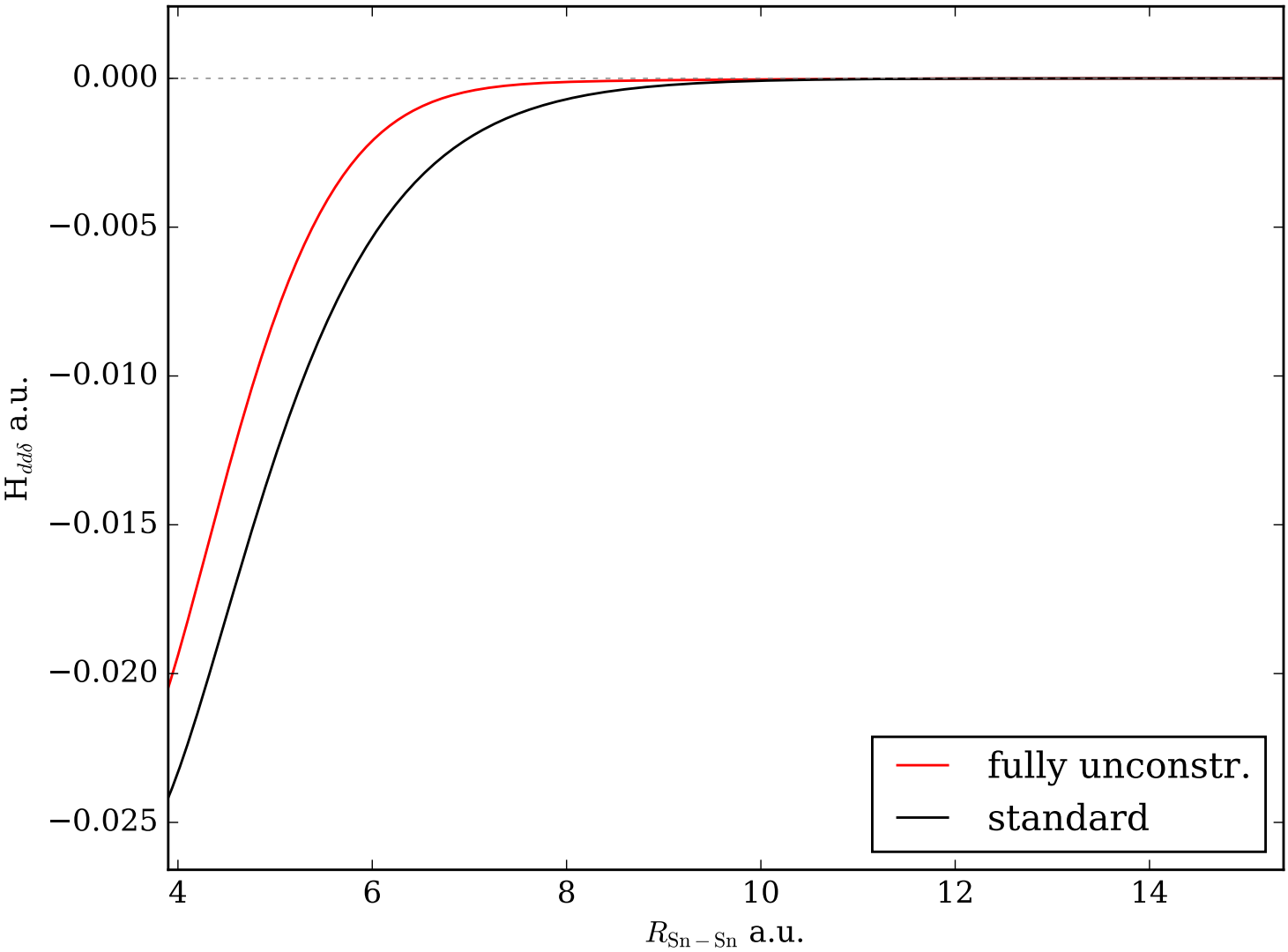


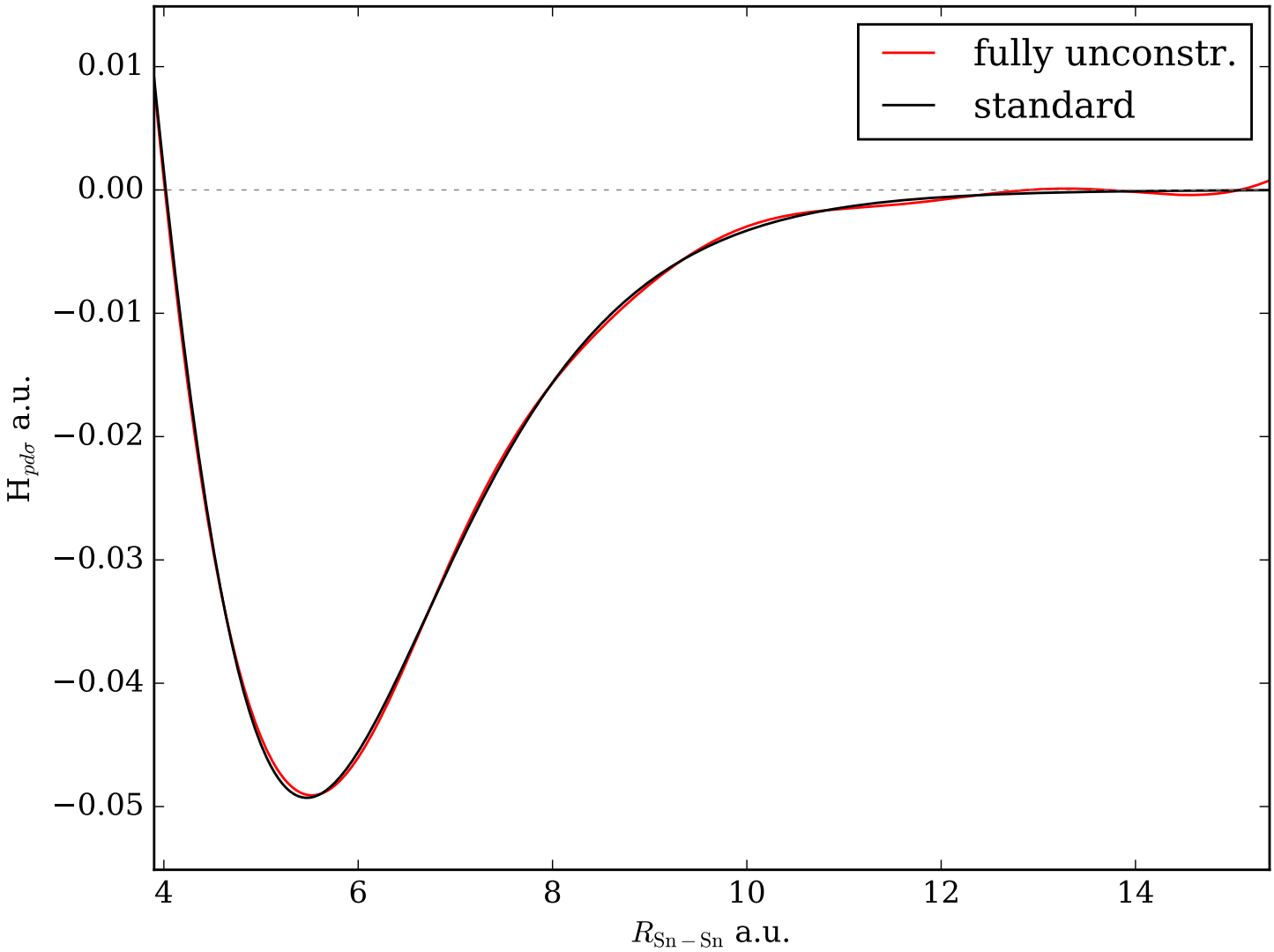
4 Sn-Sn

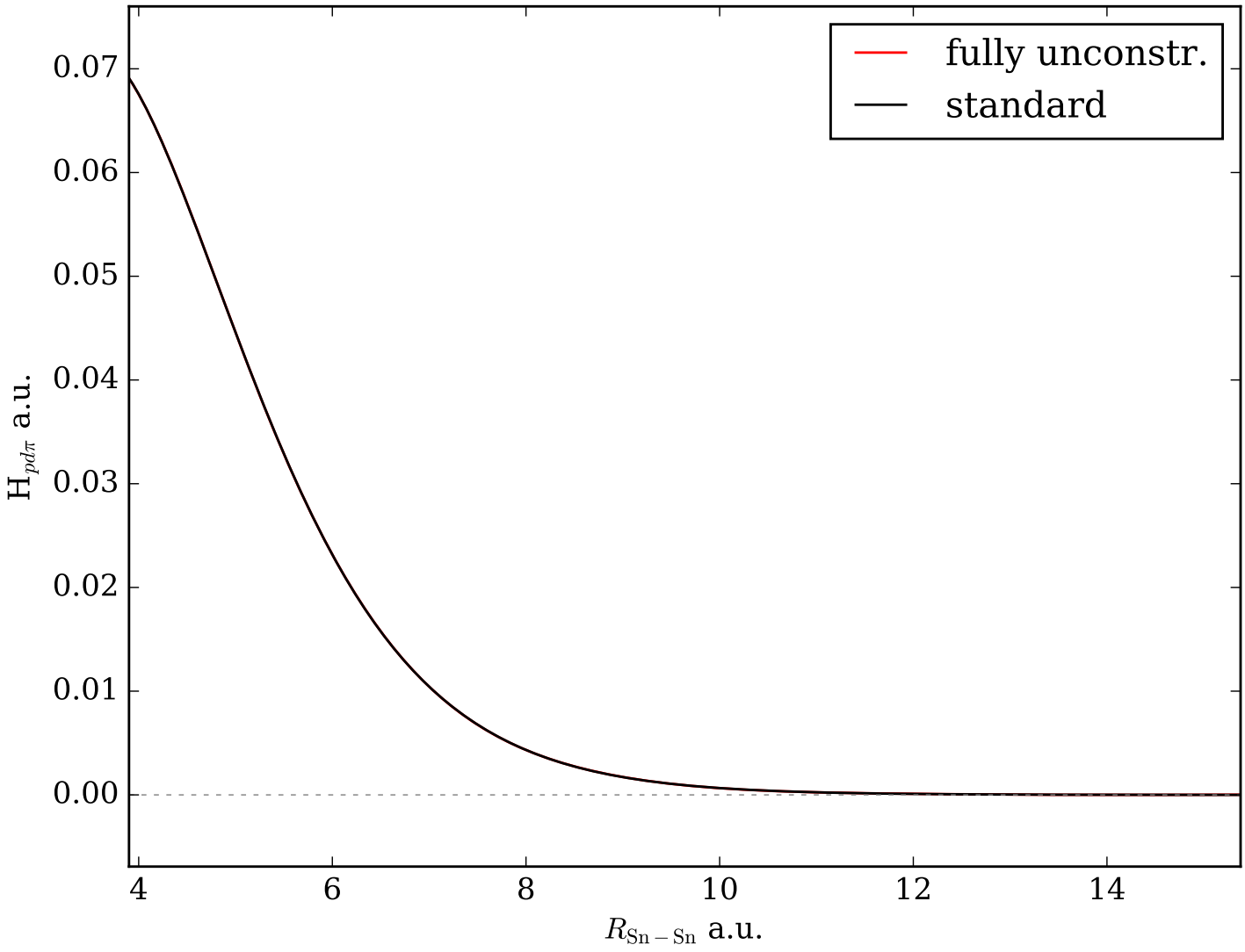
4.1 Electronic

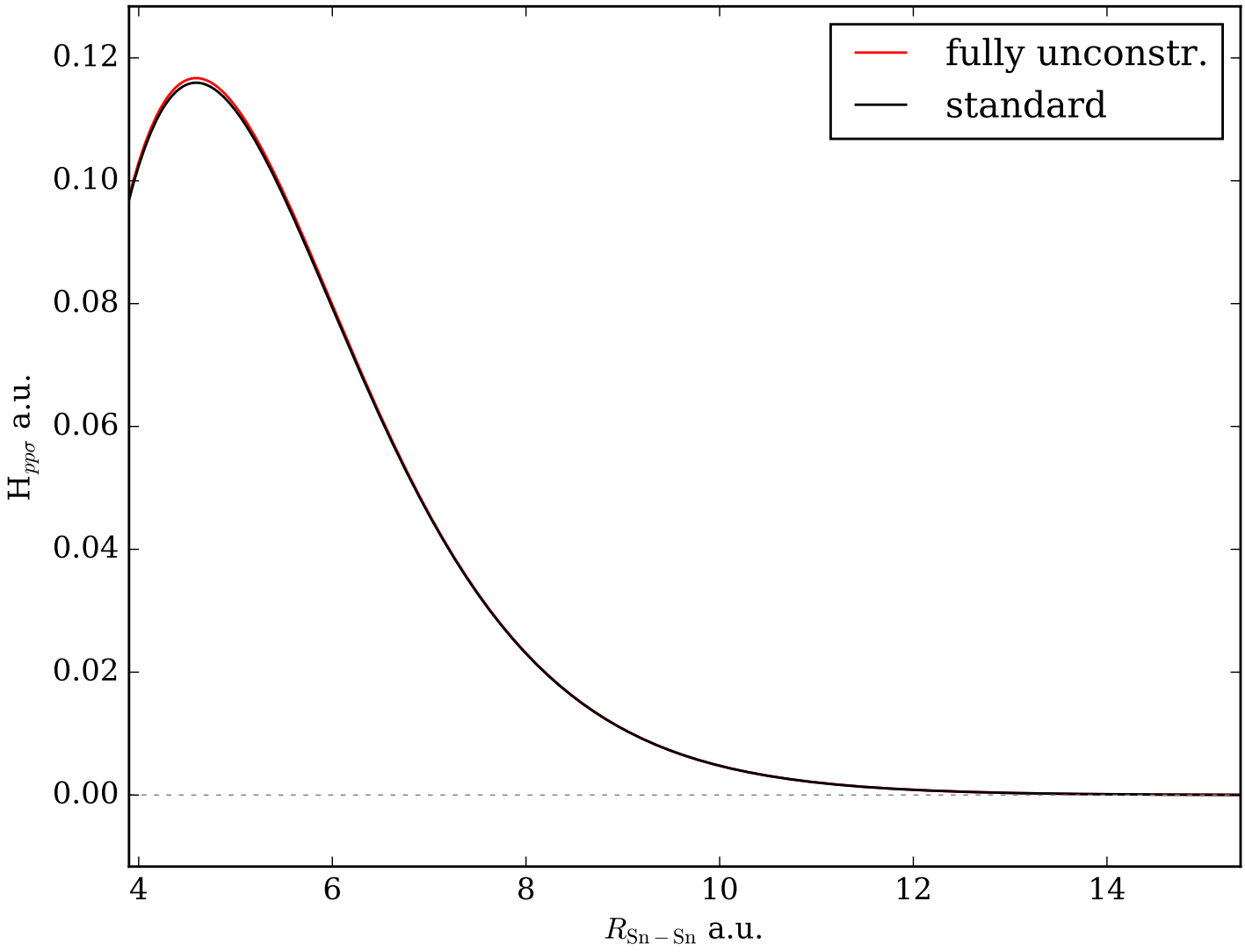


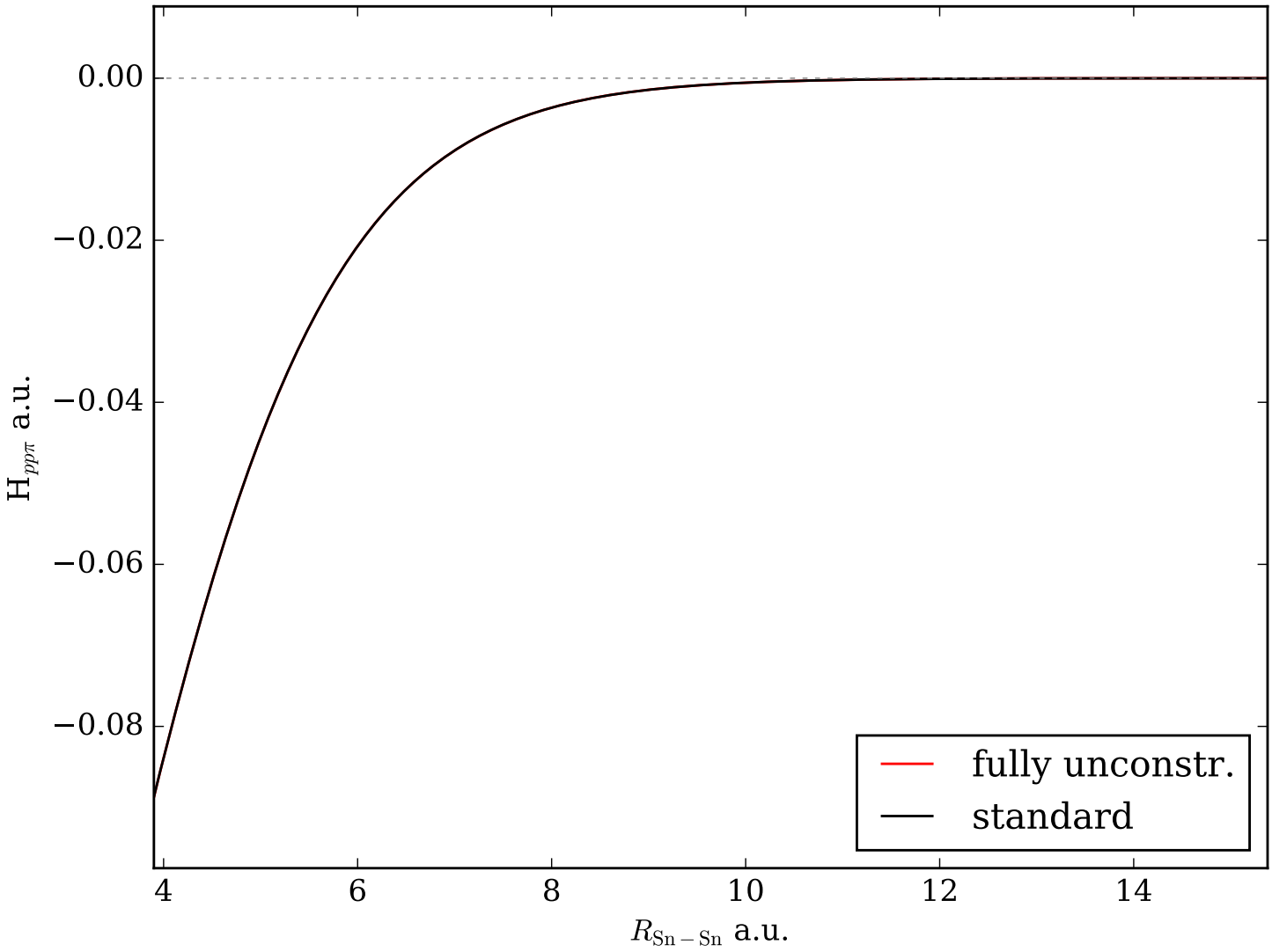

fully unconstr.
standard
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
$H_{dd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.

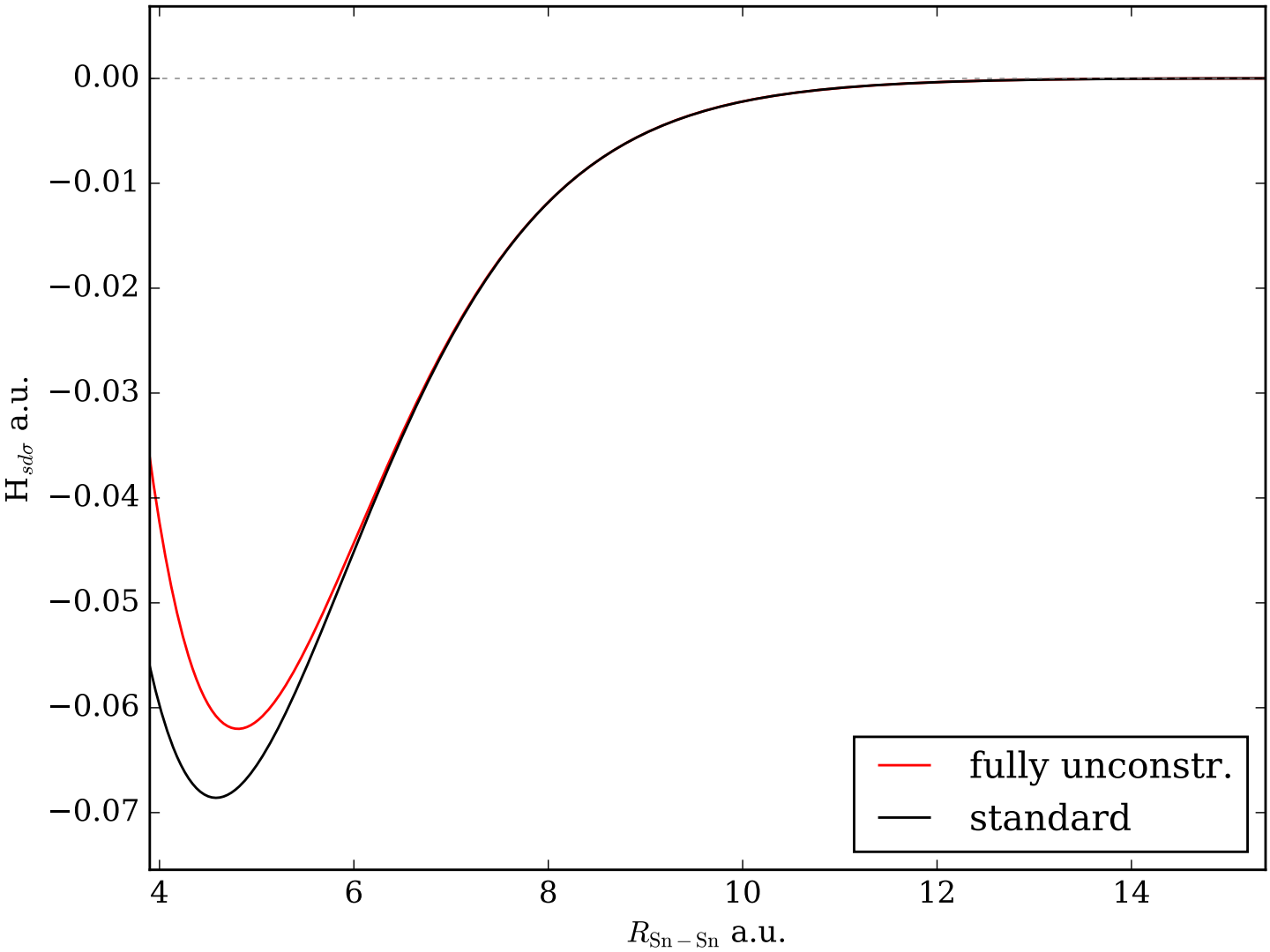

0.000
−0.005
−0.010
−0.015
−0.020
−0.025
$H_{dd\delta}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.
fully unconstr.
standard

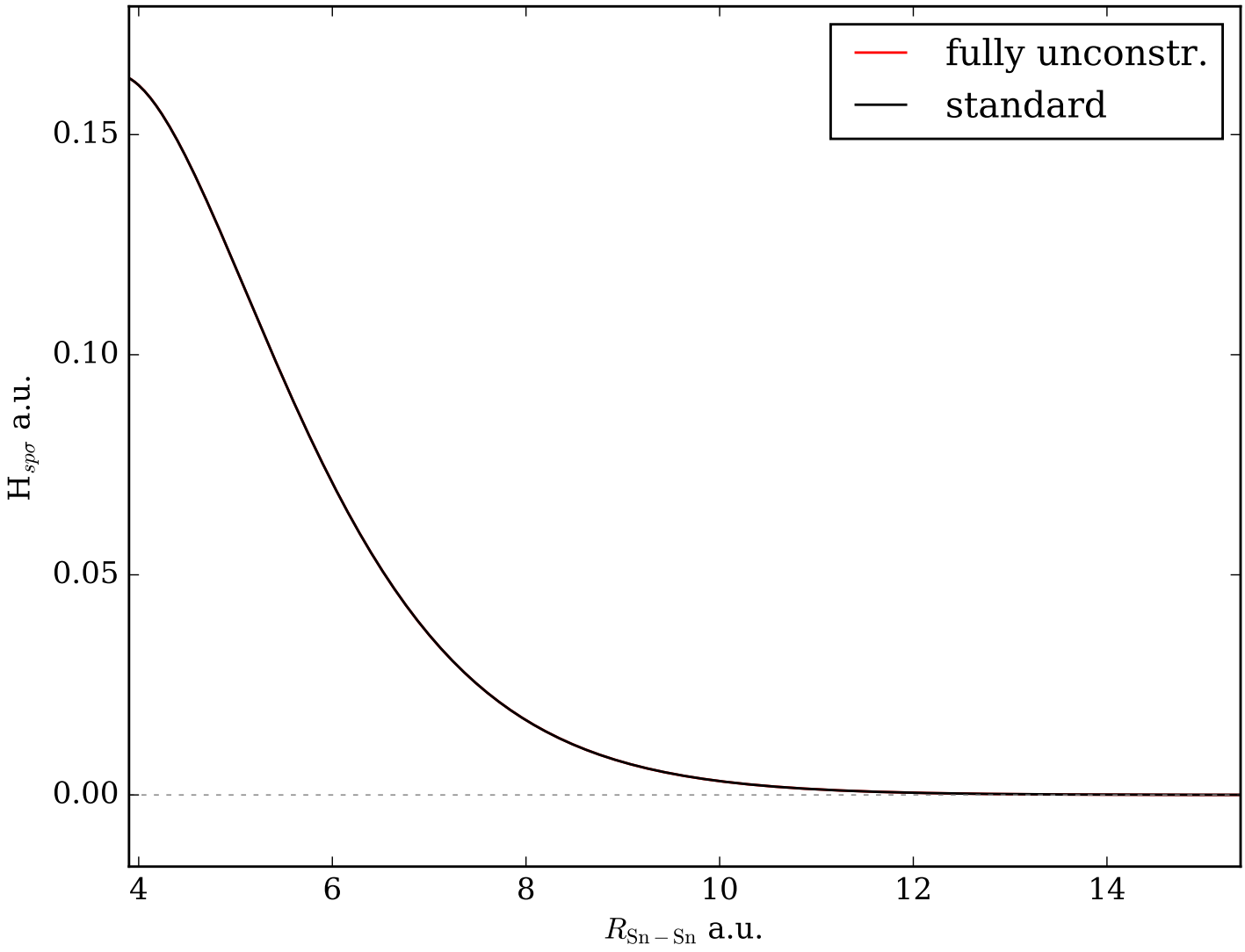

fully unconstr.
standard
0.01
0.00
−0.01
−0.02
−0.03
−0.04
−0.05
$H_{pd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.

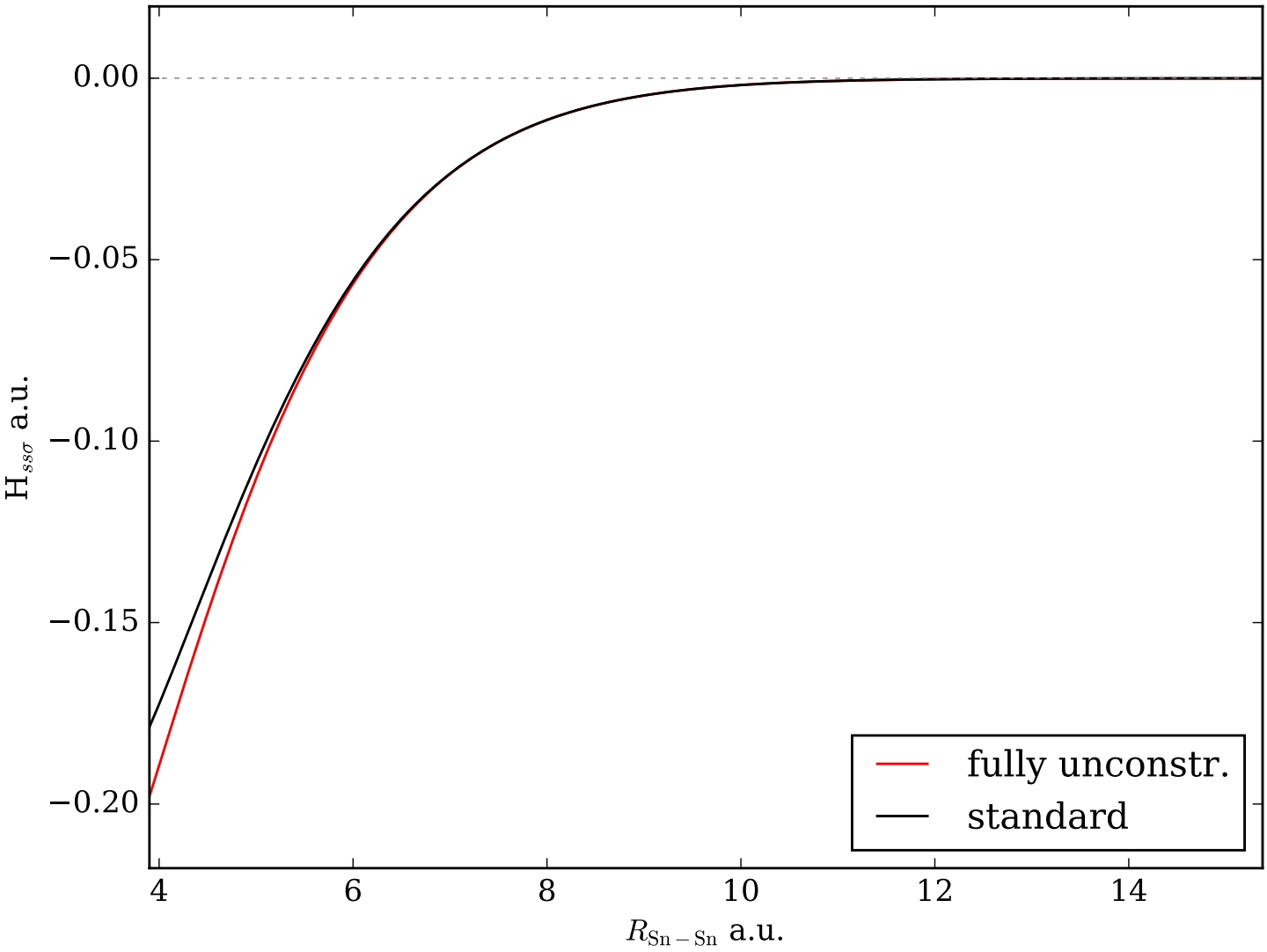

fully unconstr.
standard
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
$H_{pd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.

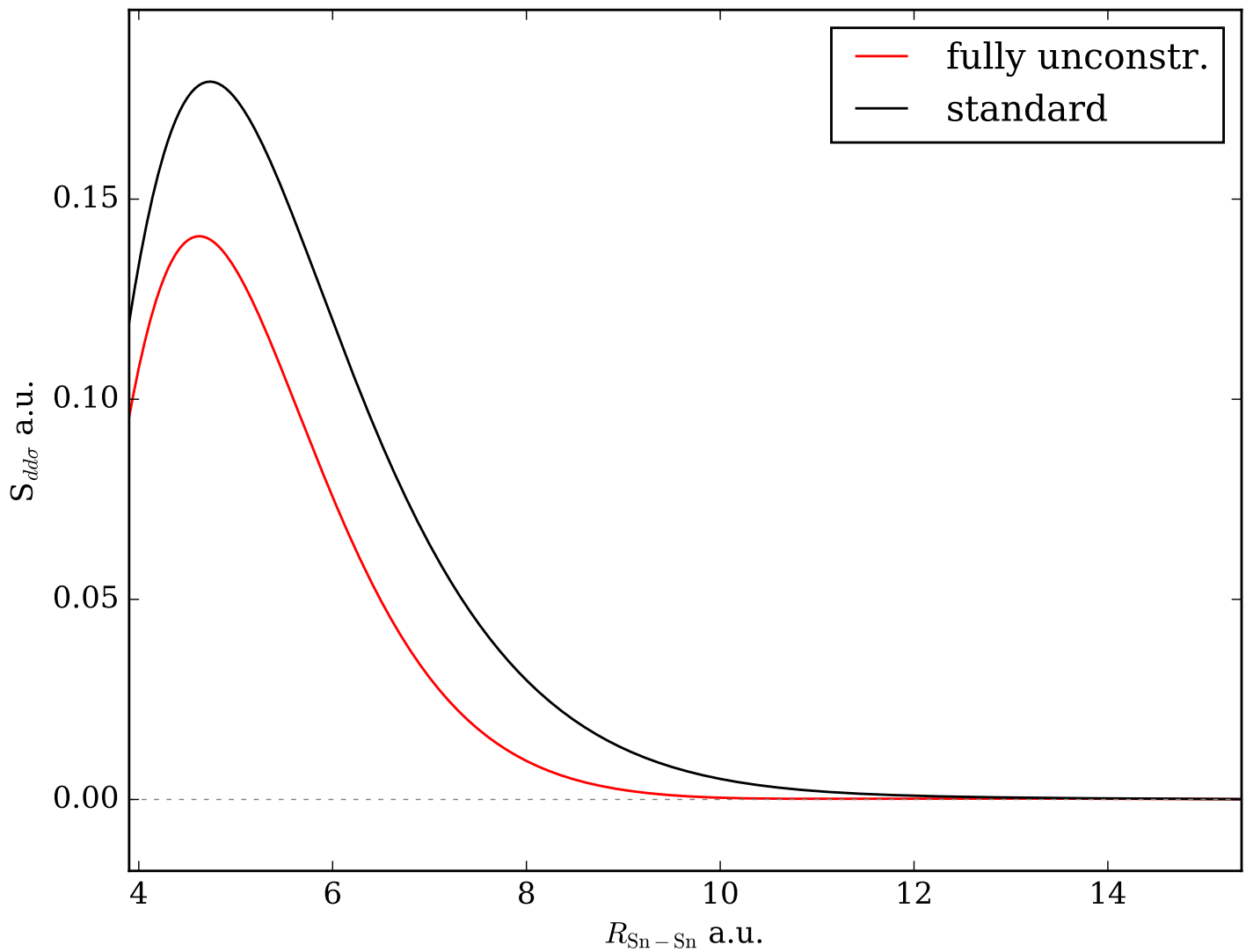

fully unconstr.
standard
0.12
0.10
0.08
0.06
0.04
0.02
0.00
$H_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.

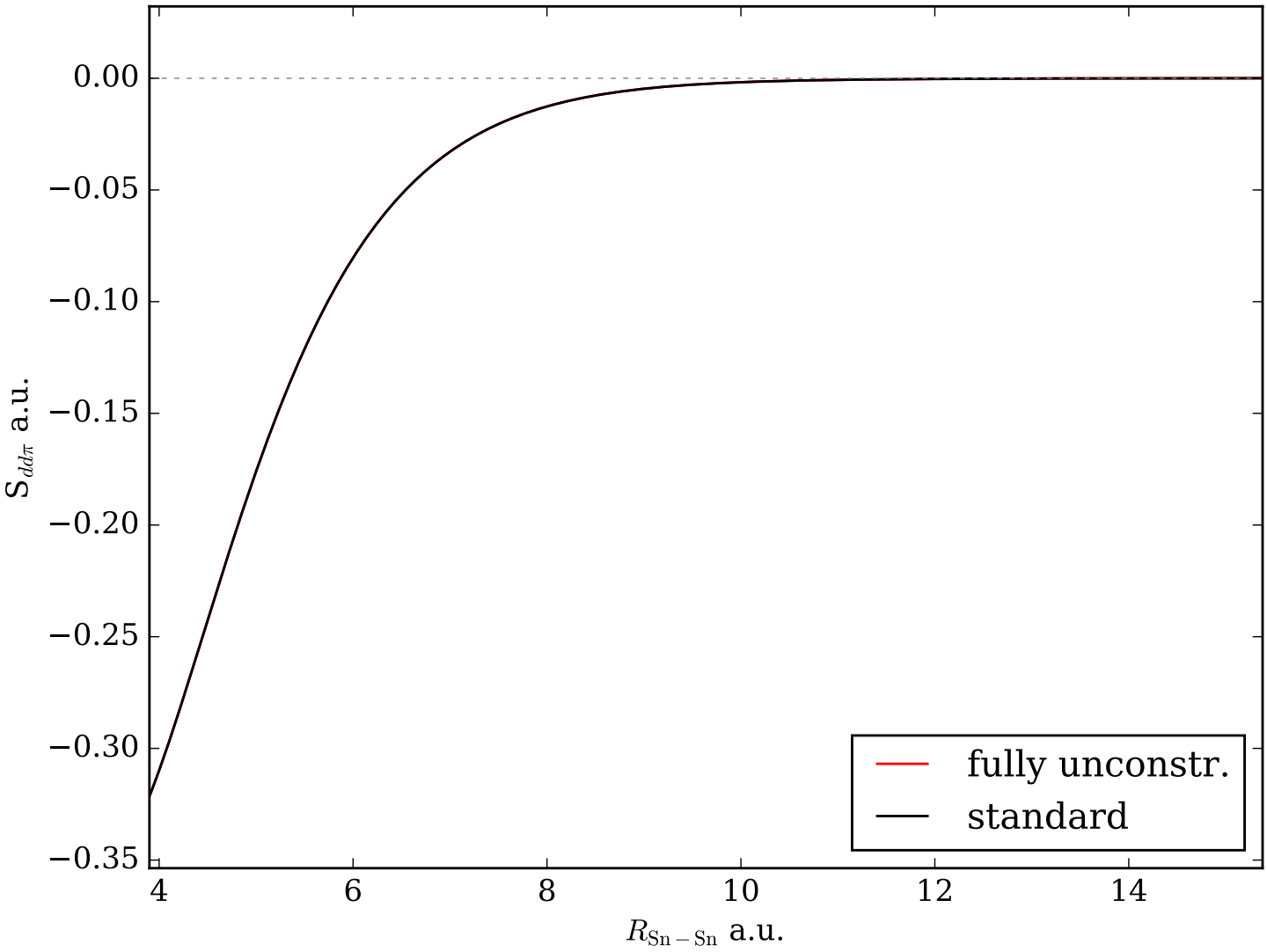

0.00
−0.02
−0.04
−0.06
−0.08
$H_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.
fully unconstr.
standard

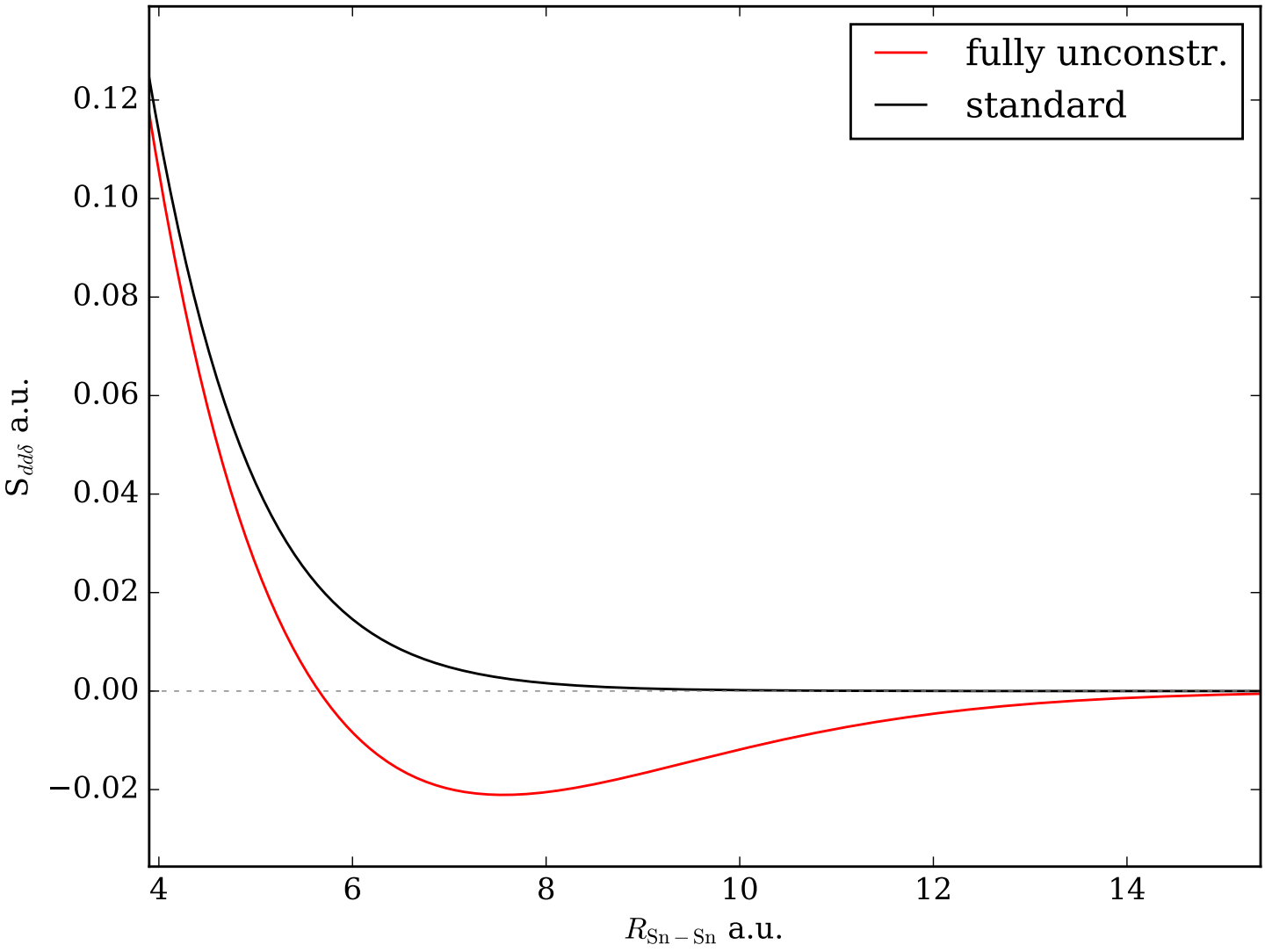

0.00
−0.01
−0.02
−0.03
−0.04
−0.05
−0.06
−0.07
$H_{sd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.
fully unconstr.
standard

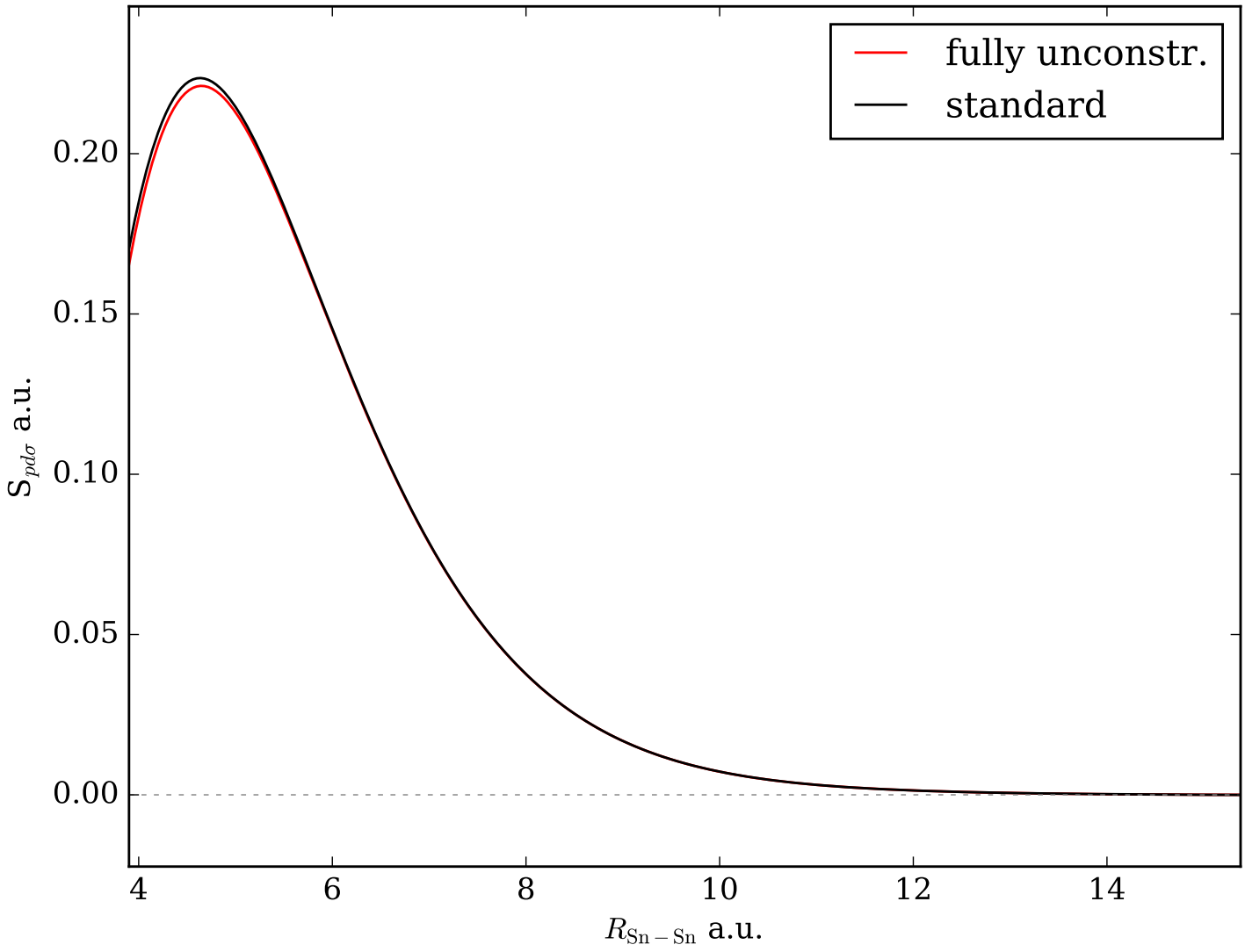

fully unconstr.
standard
0.15
0.10
0.05
0.00
$H_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.

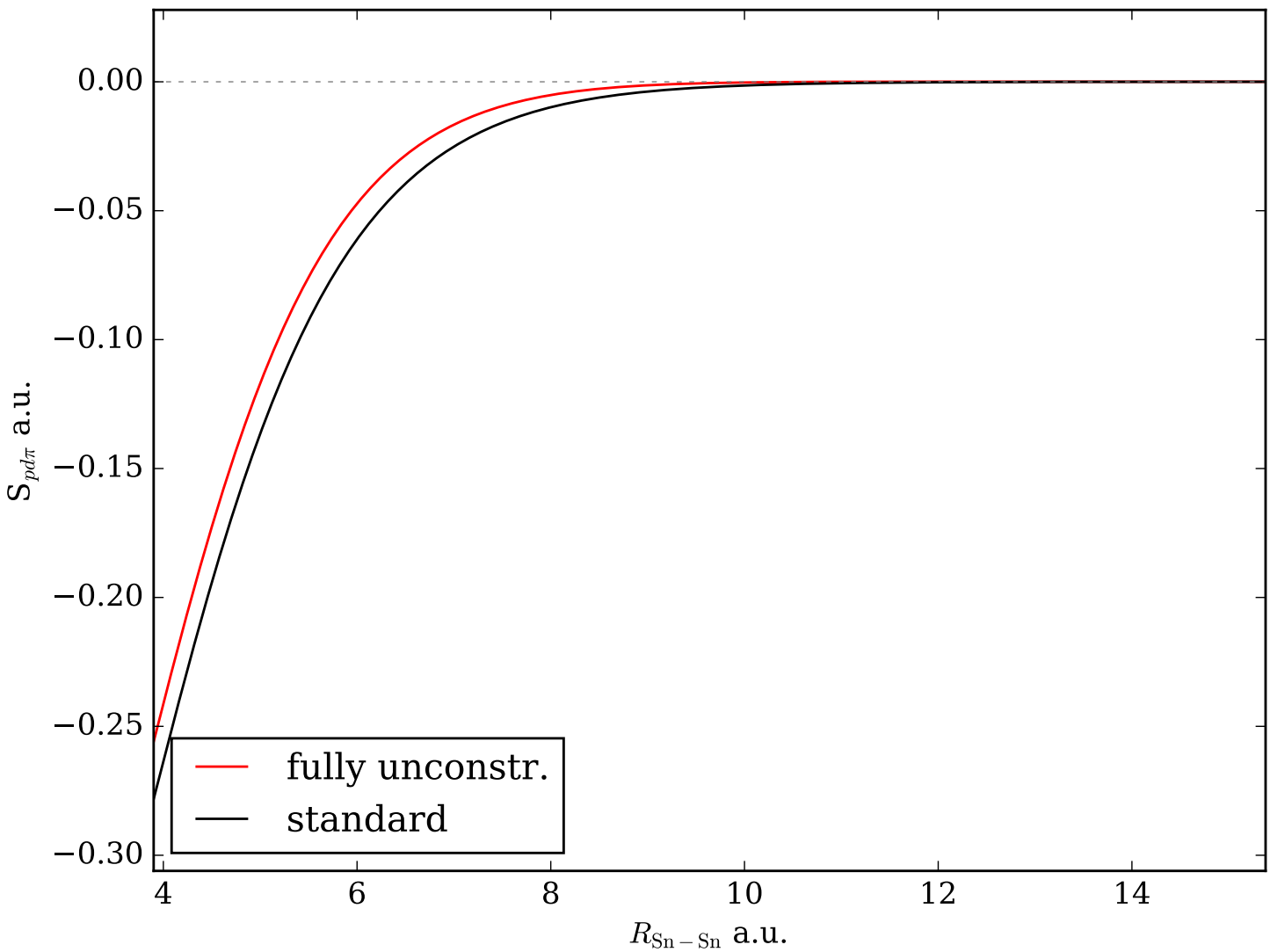

0.00
−0.05
−0.10
−0.15
−0.20
$H_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.
fully unconstr.
standard

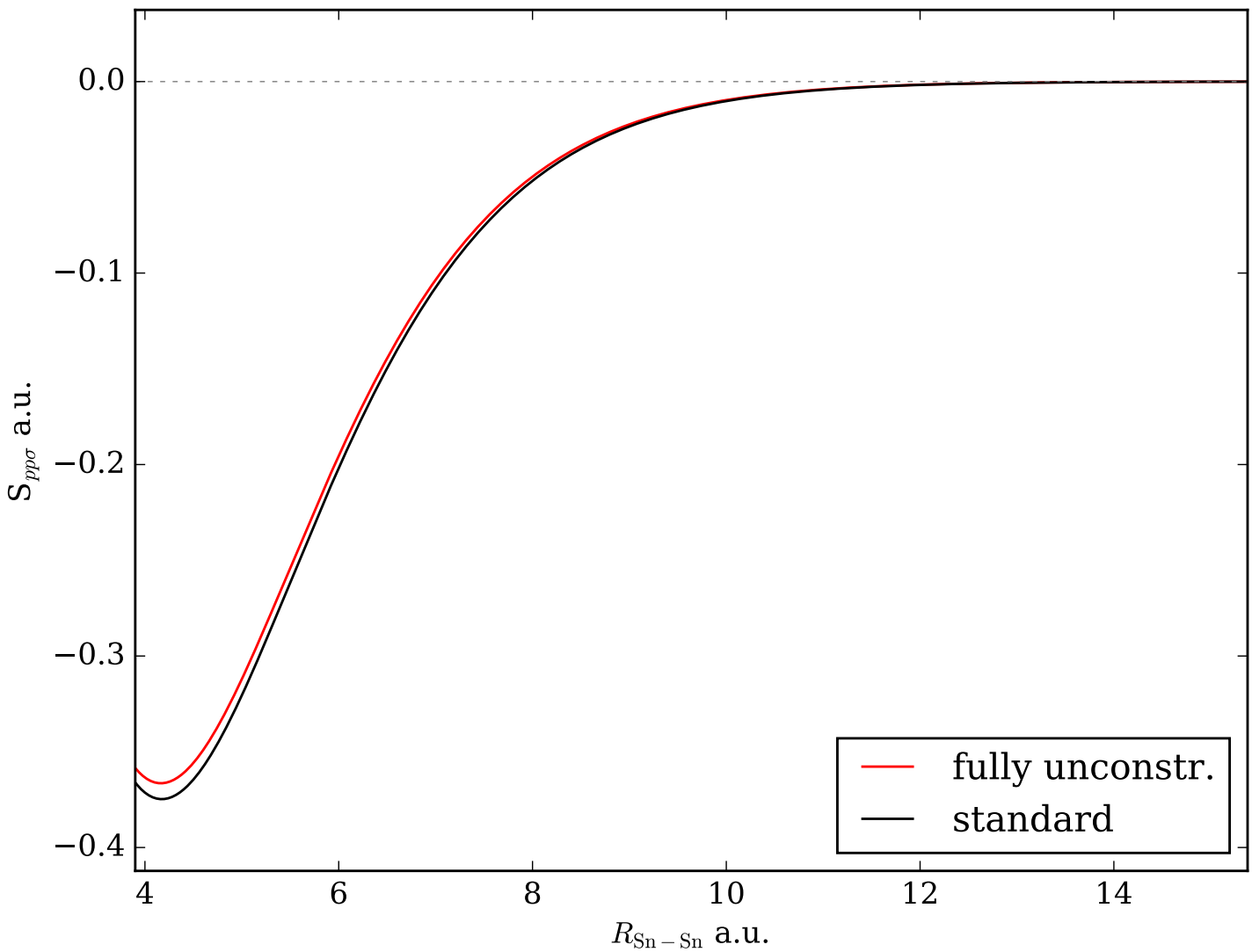

fully unconstr.
standard
0.15
0.10
0.05
0.00
$S_{dd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.

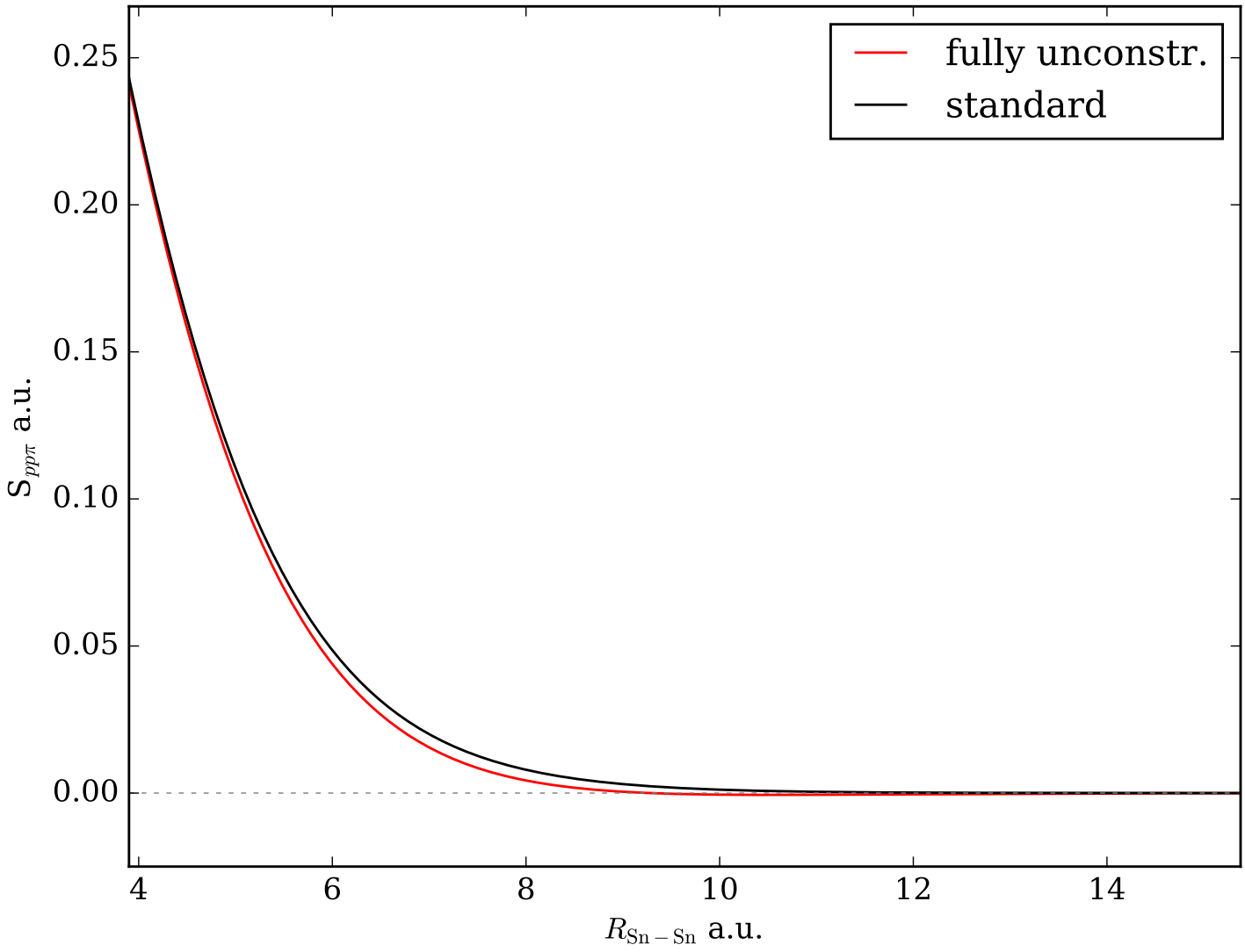

0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
−0.35
$S_{dd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.
fully unconstr.
standard

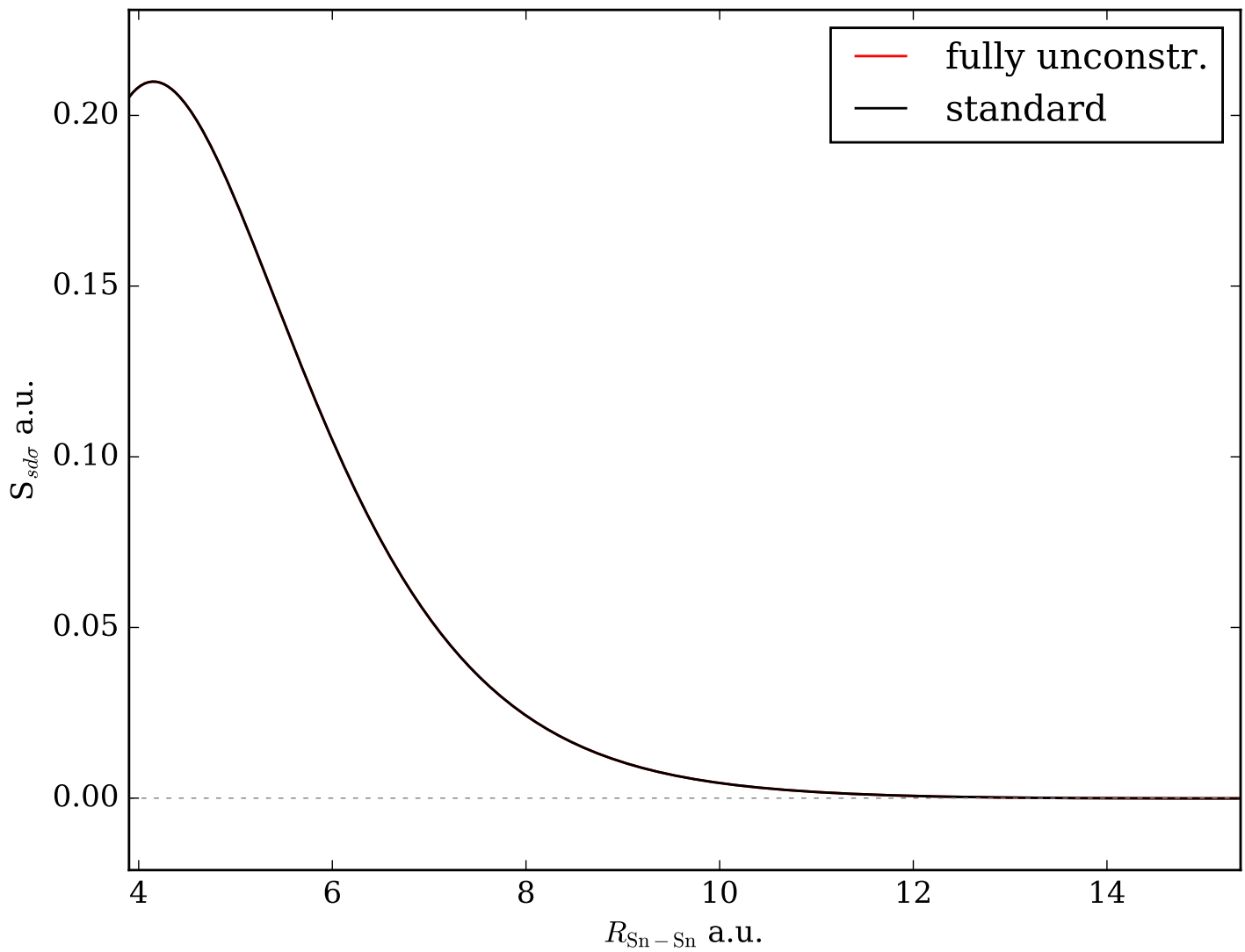

fully unconstr.
standard
0.12
0.10
0.08
0.06
0.04
0.02
0.00
−0.02
$S_{dd\delta}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.

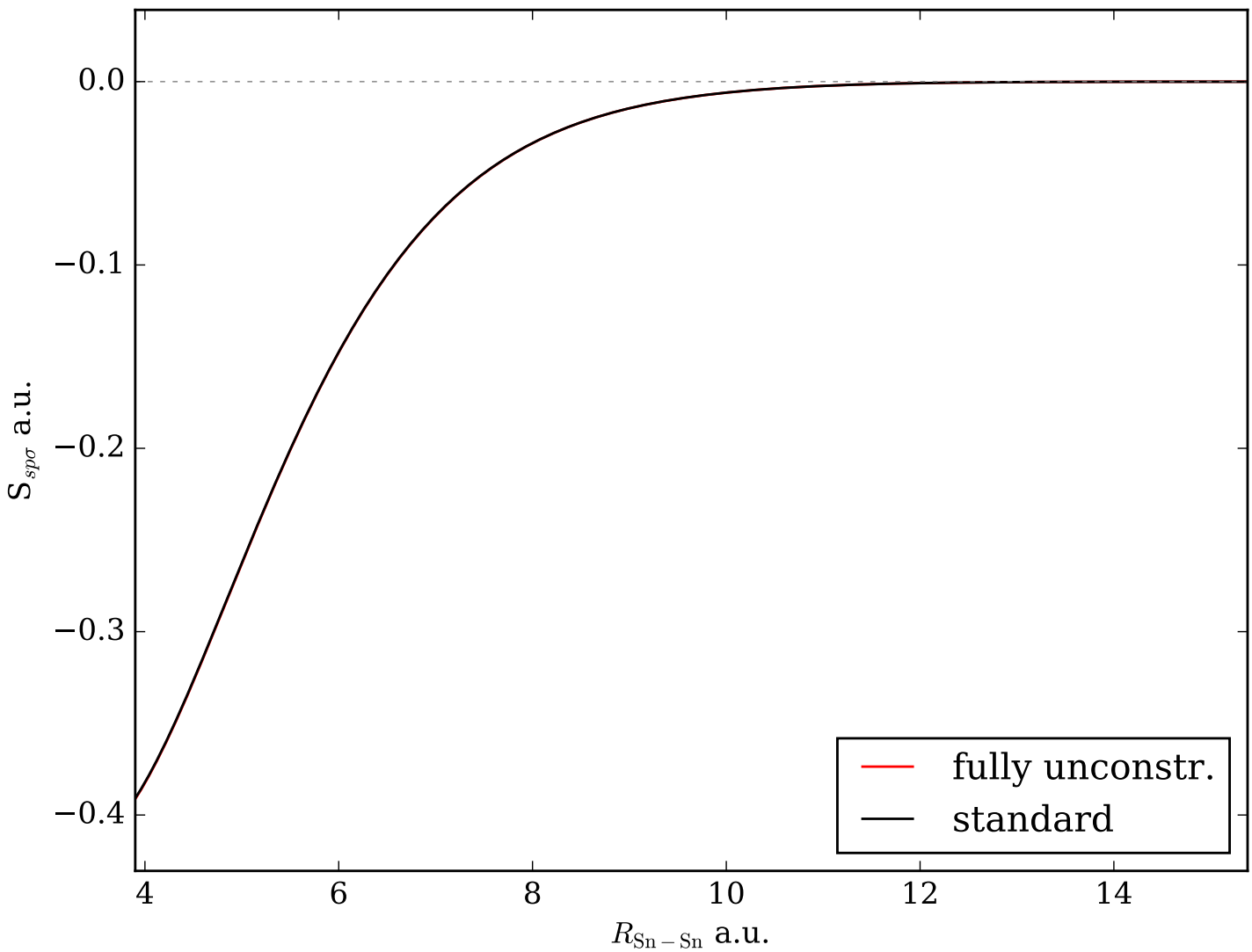

fully unconstr.
standard
0.20
0.15
0.10
0.05
0.00
$S_{pd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.

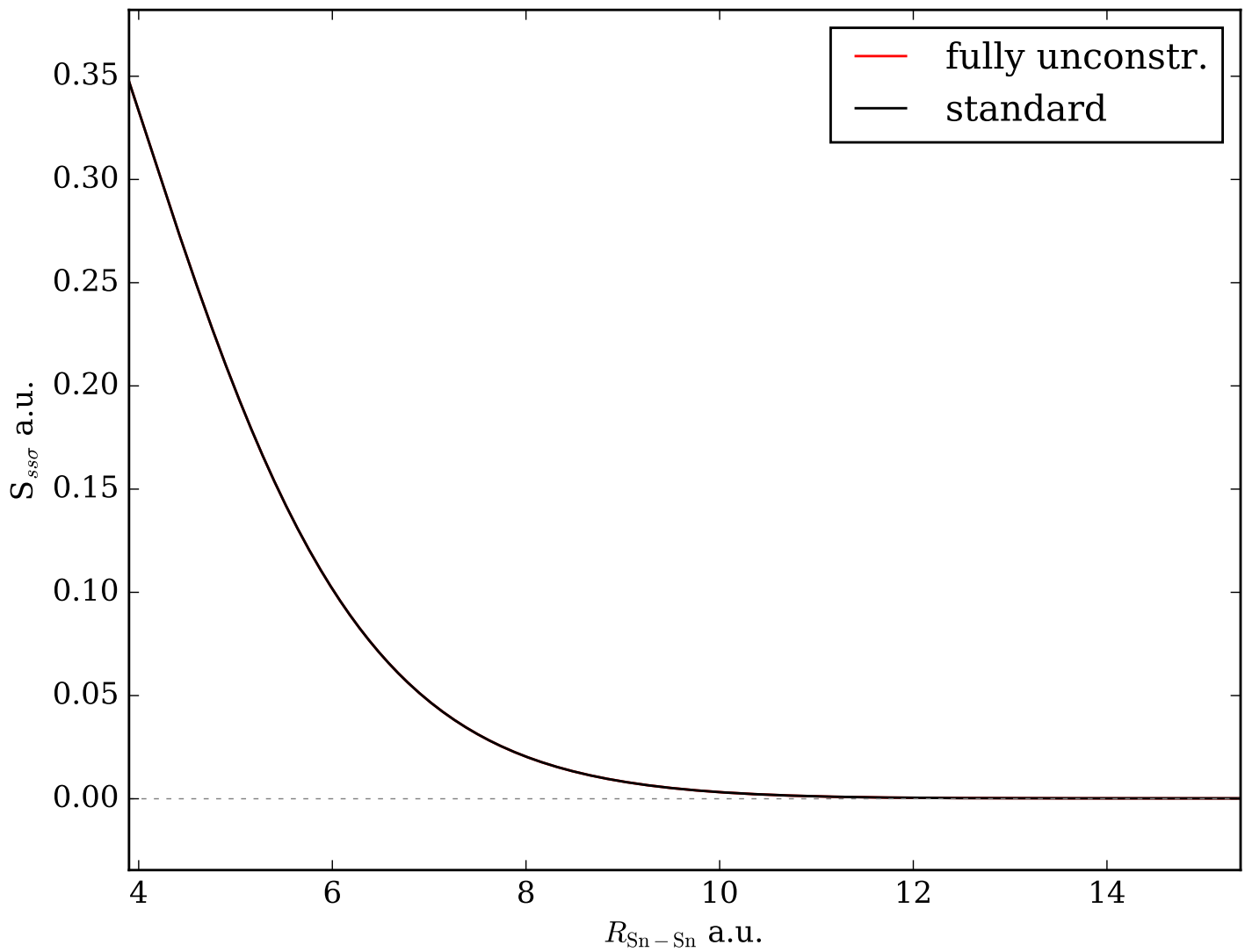

0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
$S_{pd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.
fully unconstr.
standard


0.0
−0.1
−0.2
−0.3
−0.4
$S_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.
fully unconstr.
standard

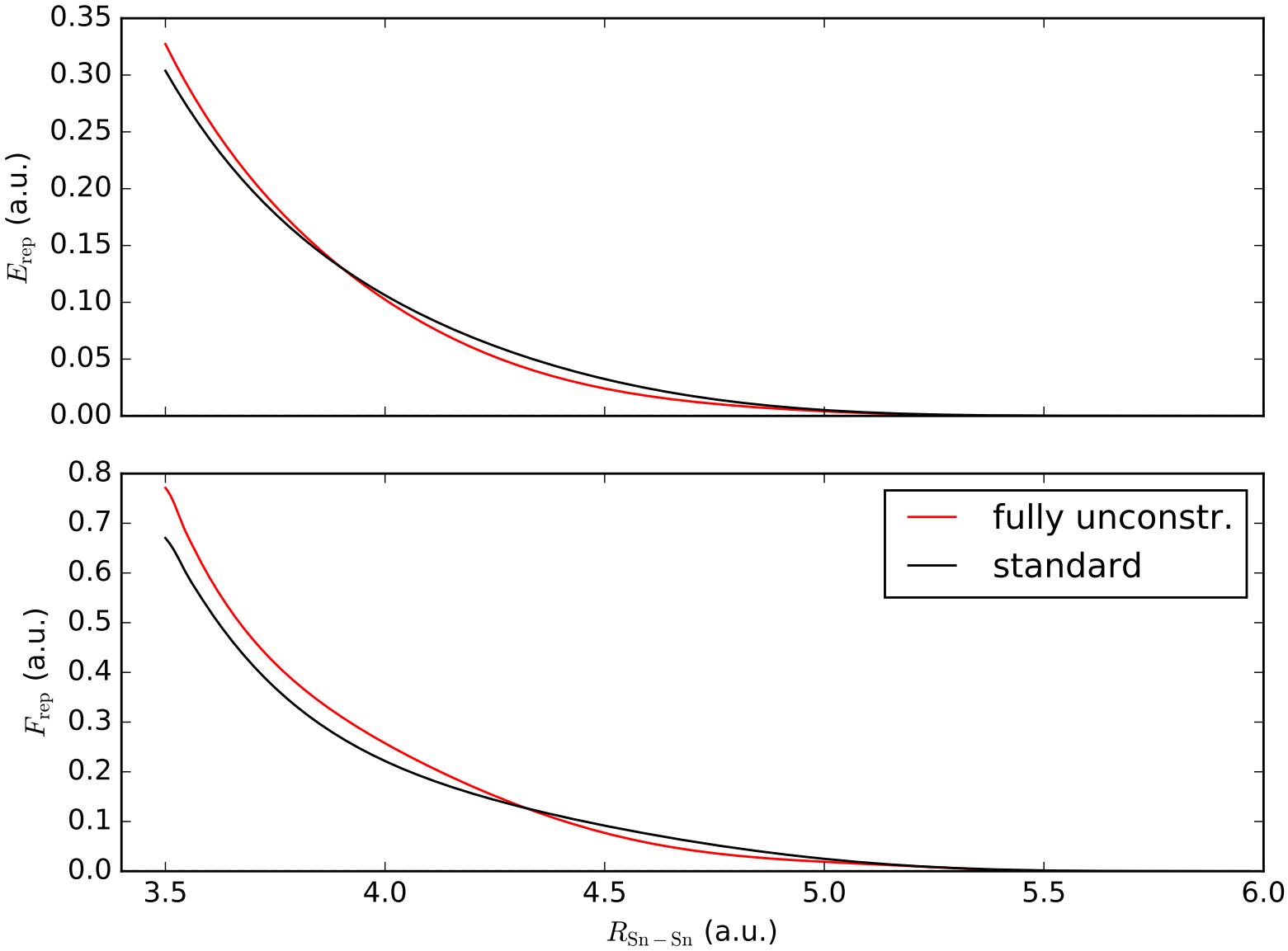

fully unconstr.
standard
0.25
0.20
0.15
0.10
0.05
0.00
$S_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.


fully unconstr.
standard
0.20
0.15
0.10
0.05
0.00
$S_{sd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.


0.0
−0.1
−0.2
−0.3
−0.4
$S_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.
fully unconstr.
standard

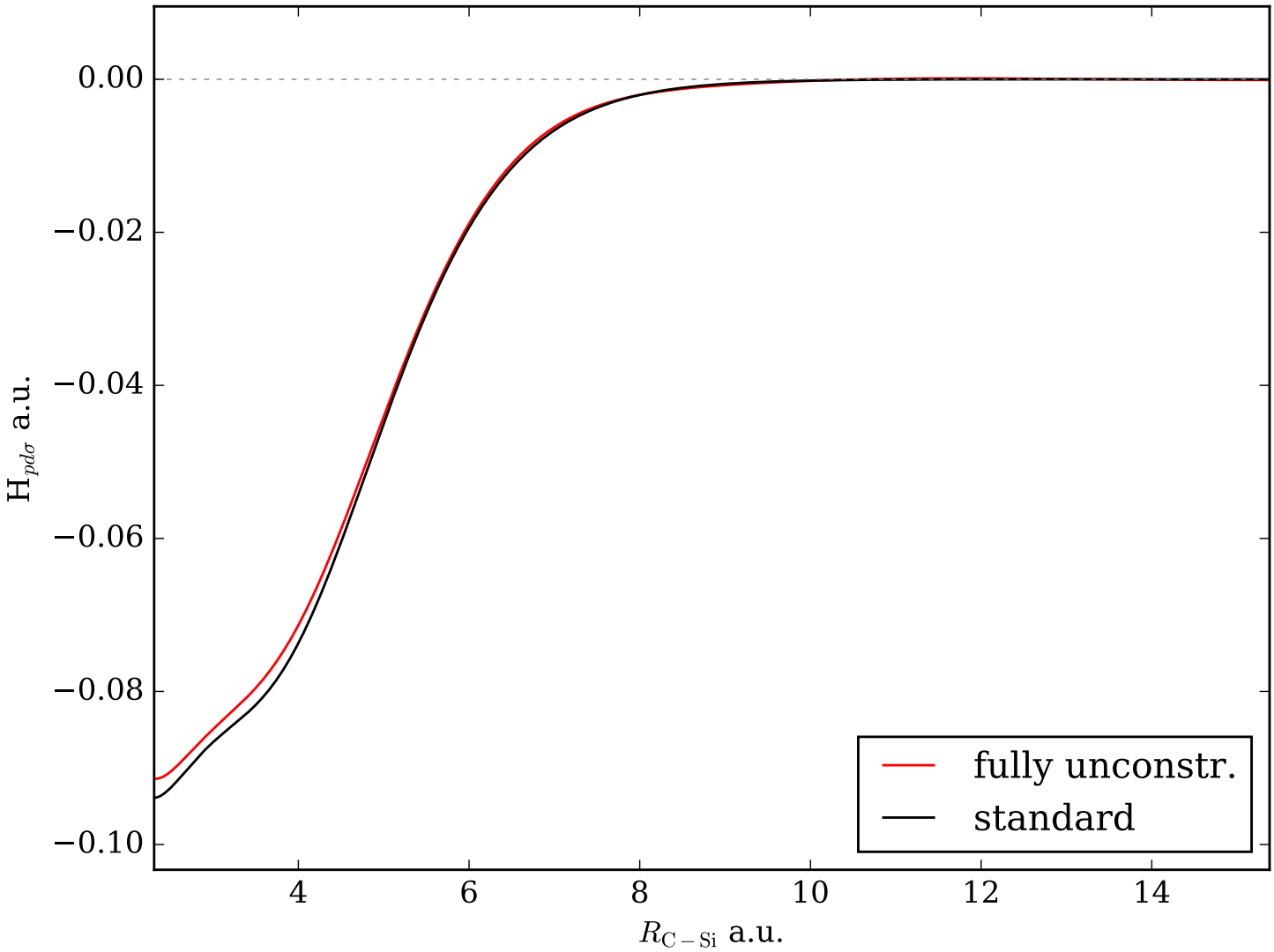

fully unconstr.
standard
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$S_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Sn}}$ a.u.

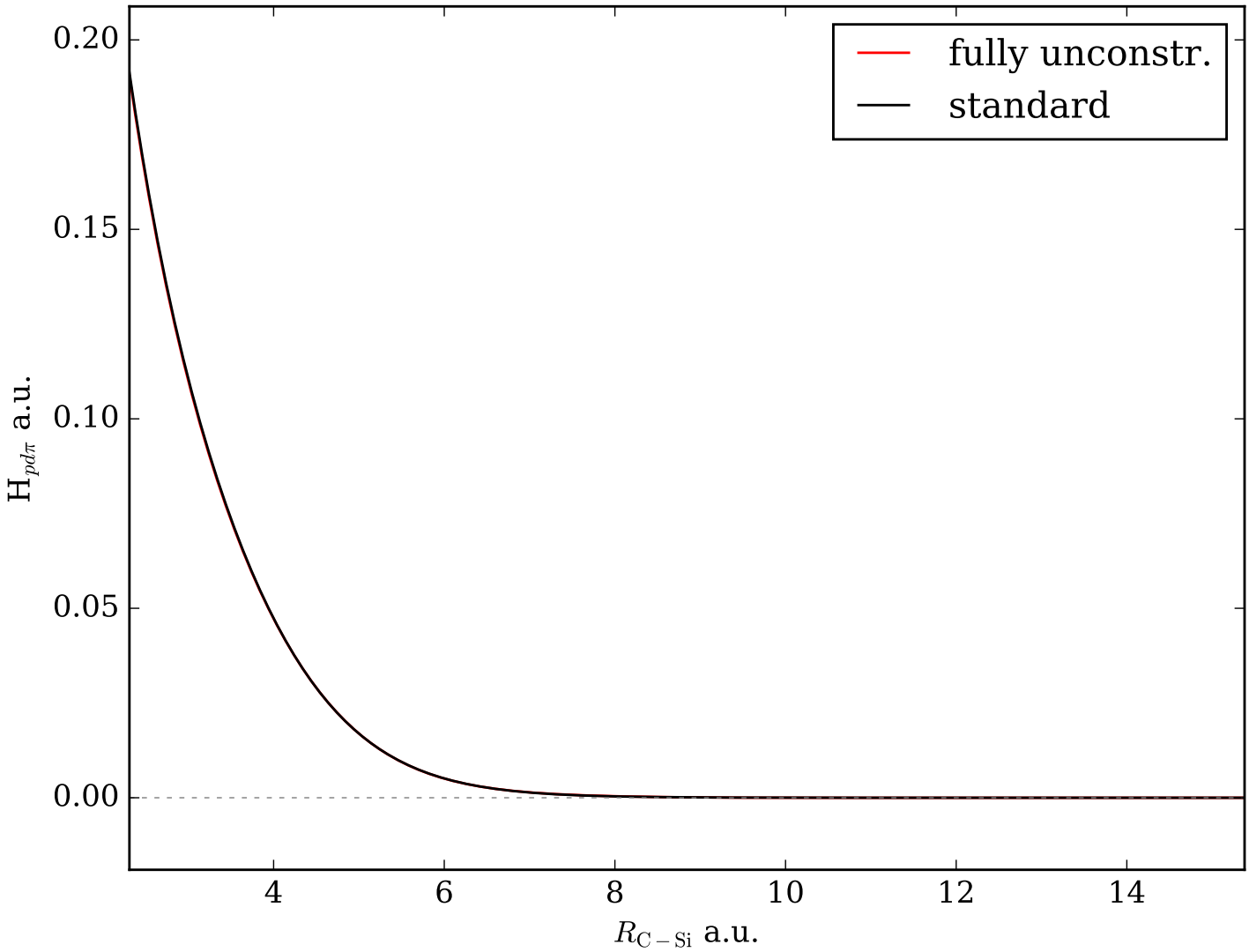
4.2 Repulsive

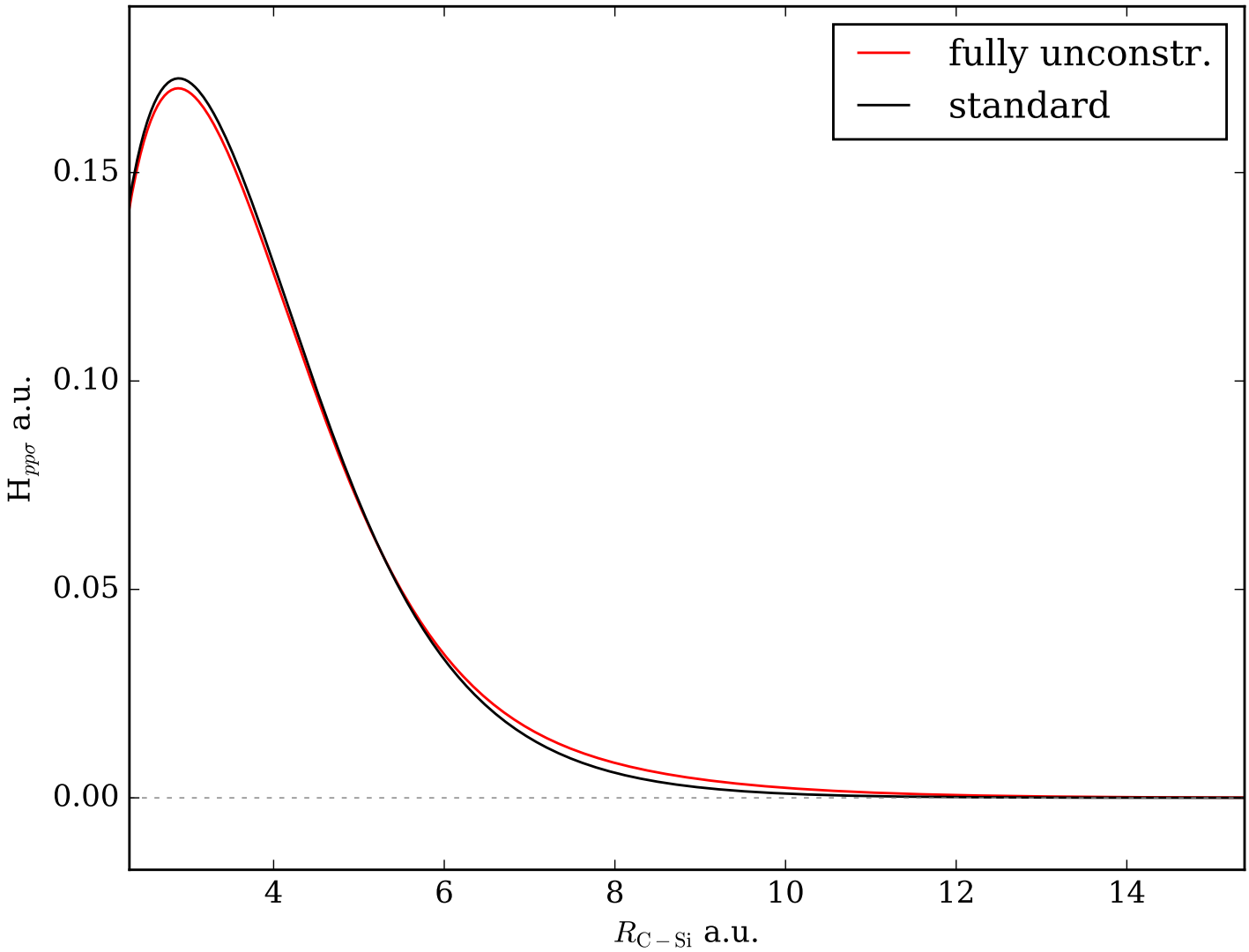


5 C-Si

5.1 Electronic




fully unconstr.
standard
0.20
0.15
0.10
0.05
0.00
$H_{pd\pi}$ a.u.
4
6
8
10
12
14
R_{C-Si} a.u.


fully unconstr.
standard
0.15
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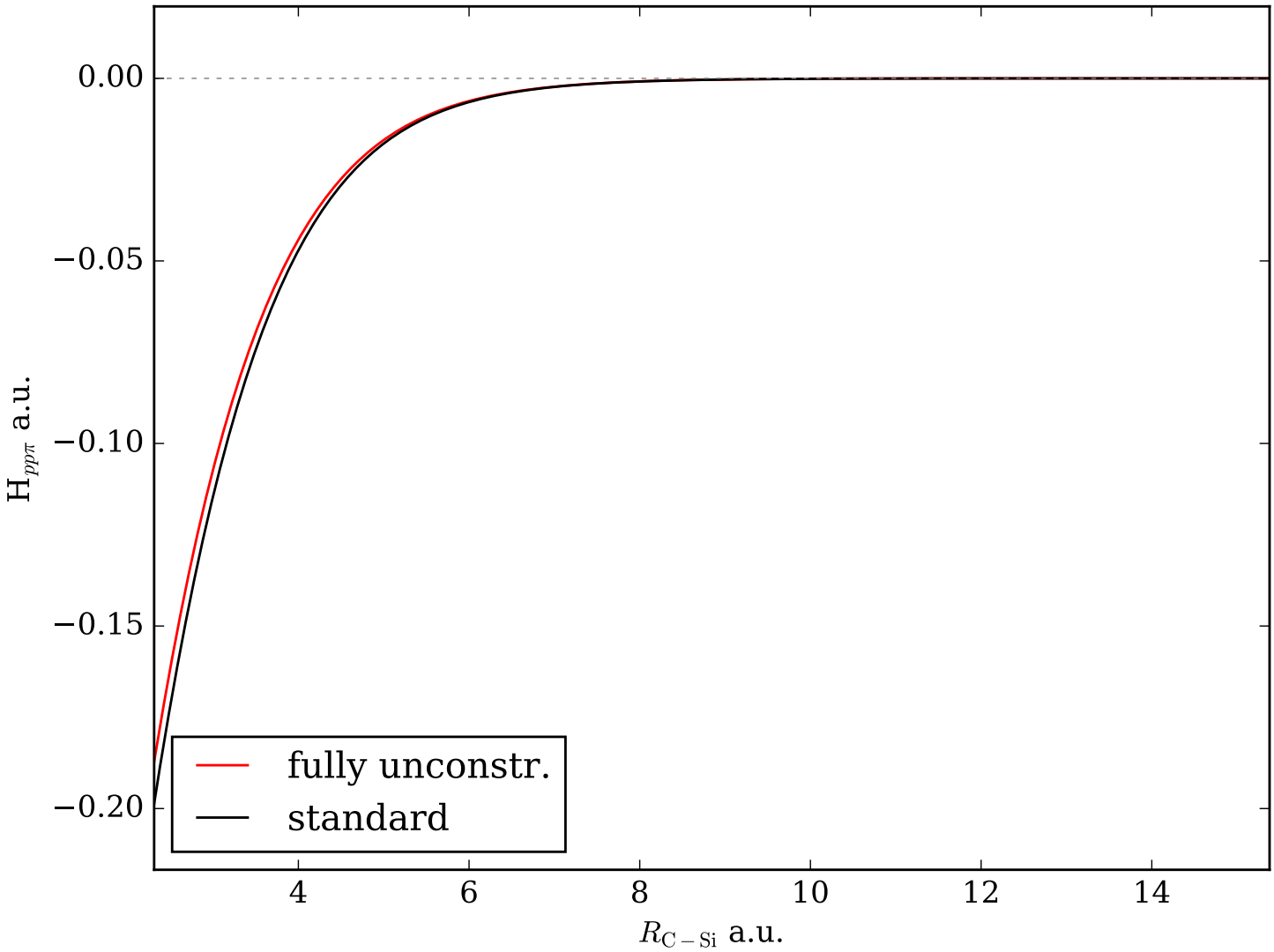
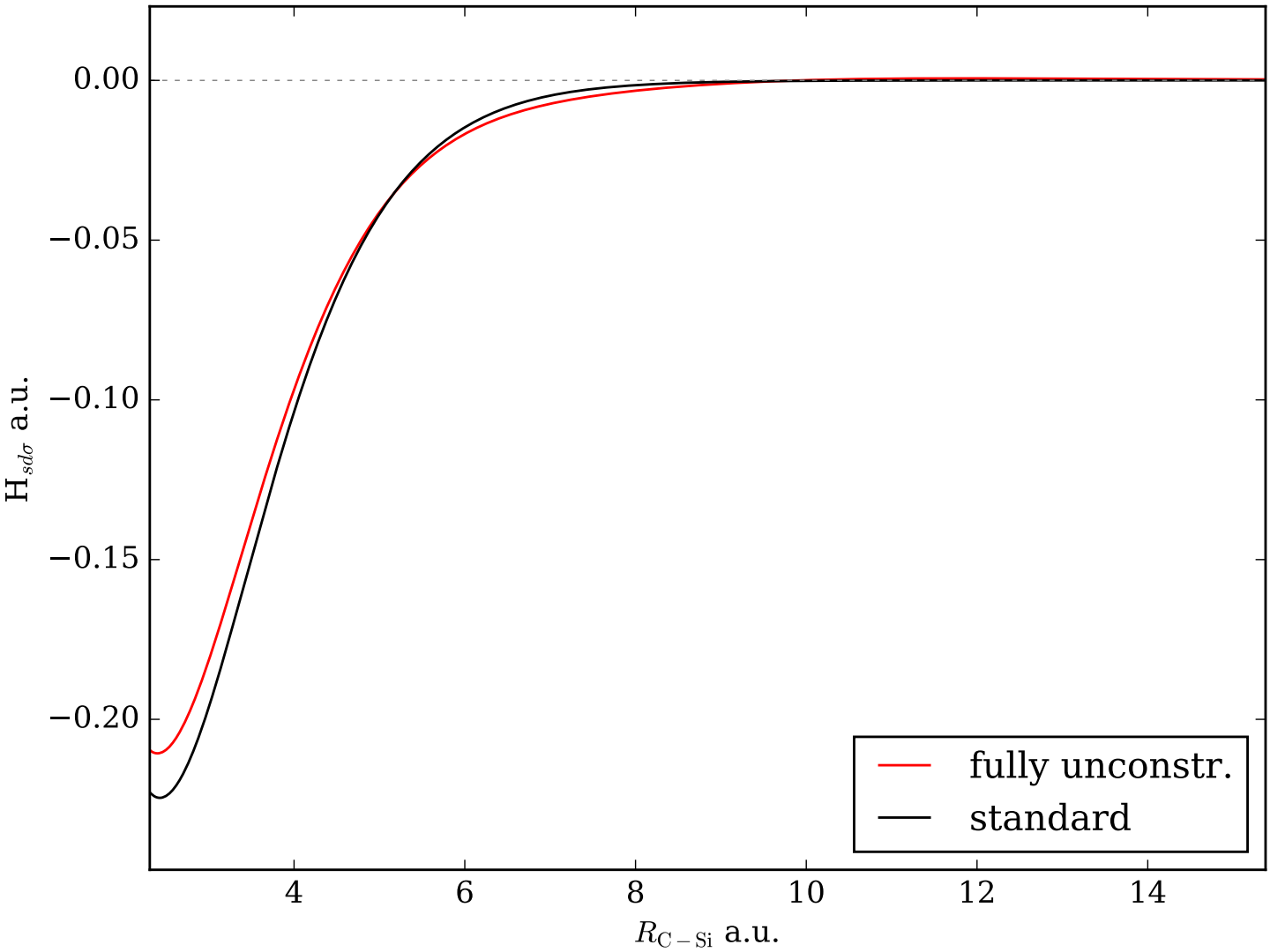
0.05
0.00
$H_{pp\sigma}$ a.u.
4
6
8
10
12
14
R_{C-Si} a.u.


0.00
−0.05
−0.10
−0.15
−0.20
$H_{pp\pi}$ a.u.
4
6
8
10
12
14
R_{C-Si} a.u.
fully unconstr.
standard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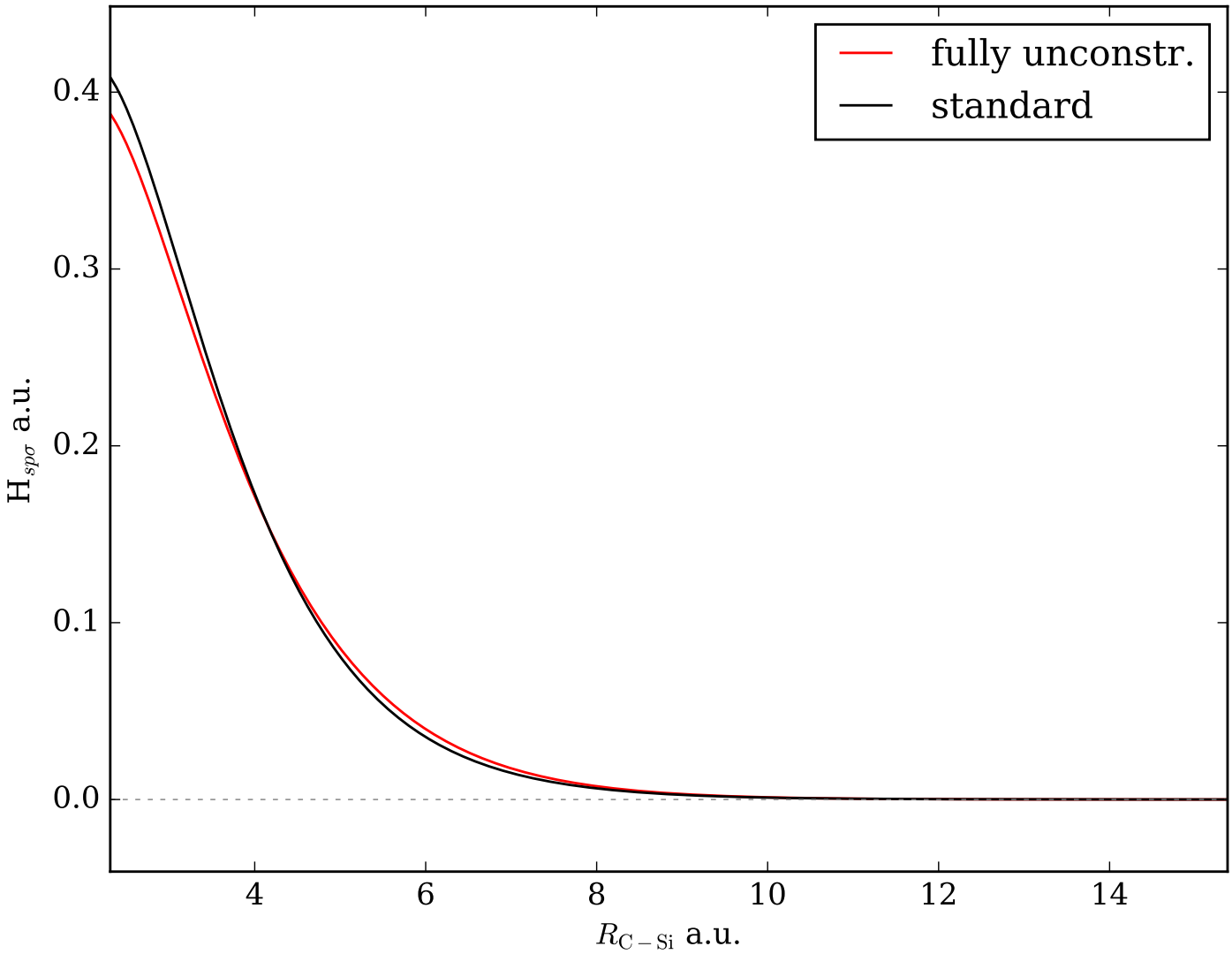
$H_{sd\sigma}$ a.u.
4
6
8
10
12
14
R_{C-Si} a.u.
fully unconstr.
standard


fully unconstr.
standard
0.4
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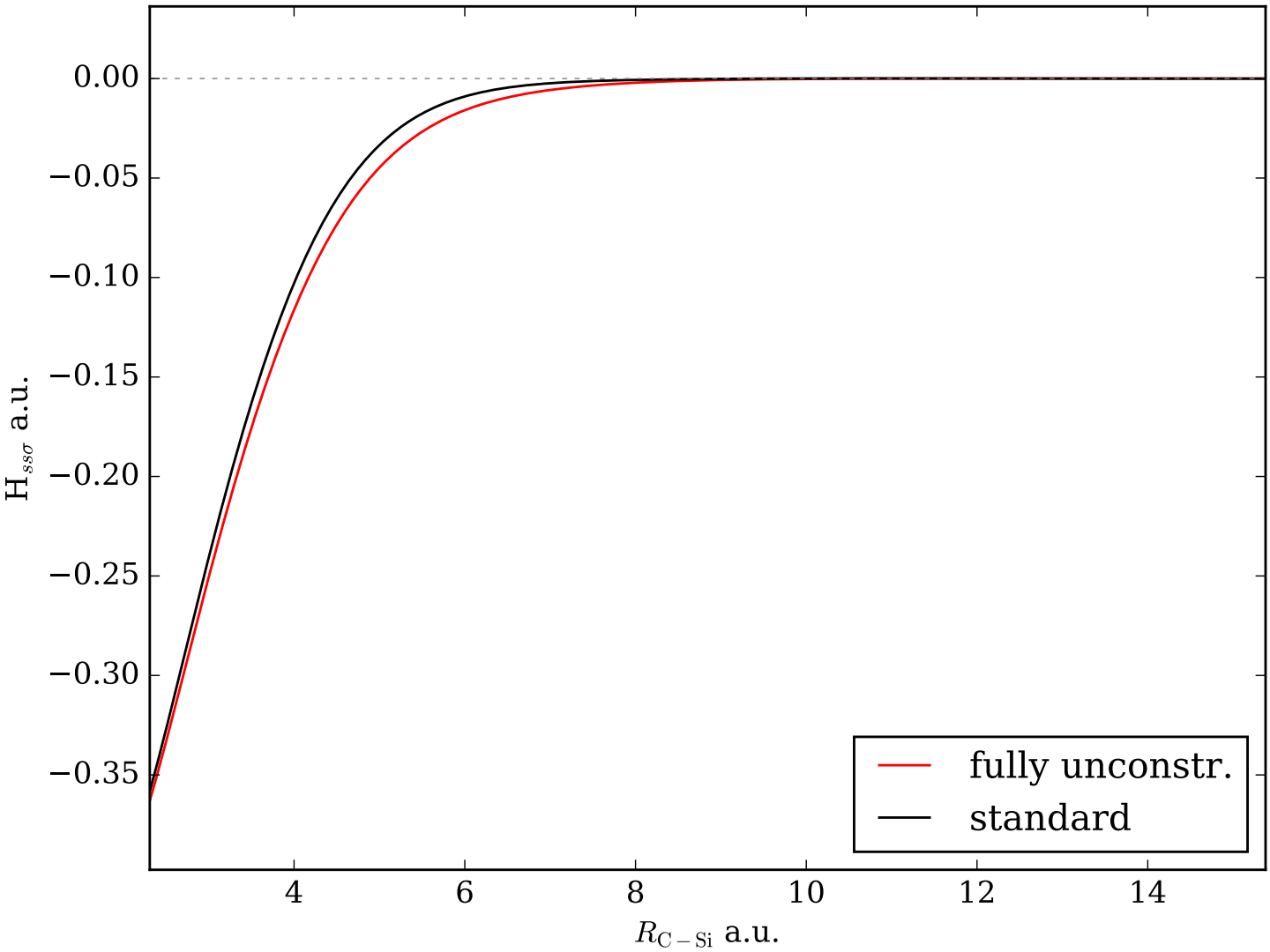
0.0
$H_{sp\sigma}$ a.u.
4
6
8
10
12
14
R_{C-Si} a.u.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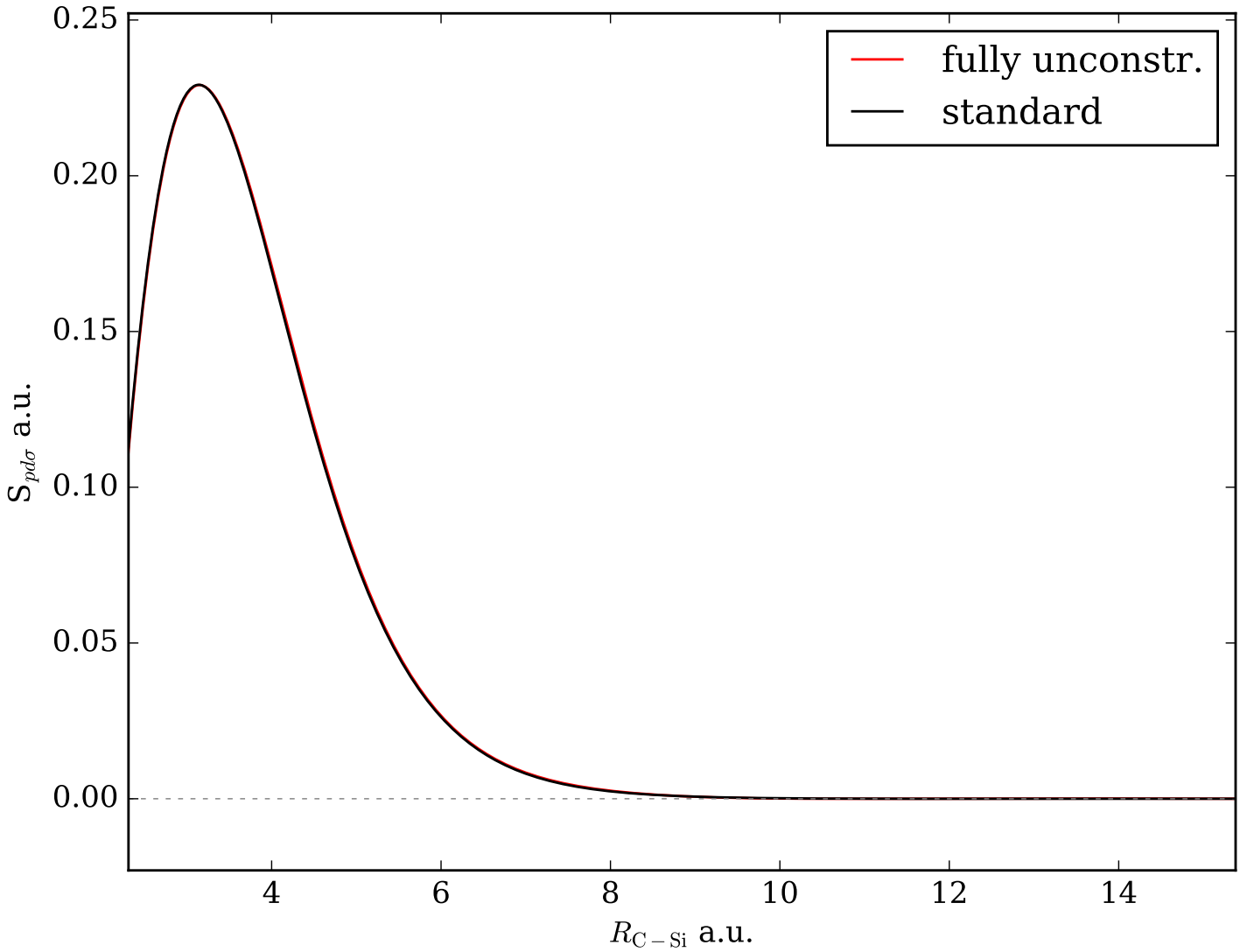
4
6
8
10
12
14
R_{C-Si} a.u.
fully unconstr.
standard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standard
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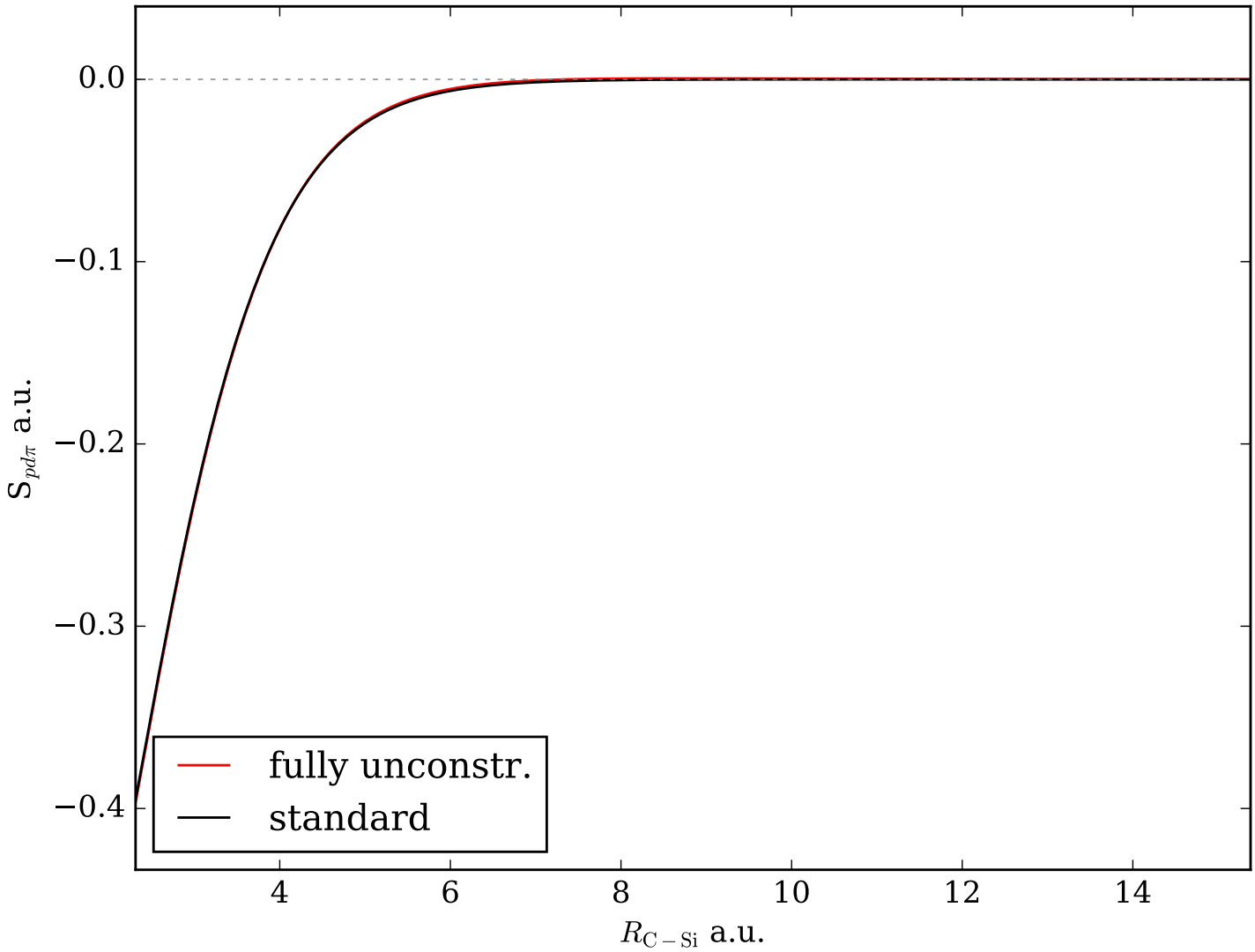
$S_{pd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Si}}$ a.u.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$S_{pd\pi}$ a.u.
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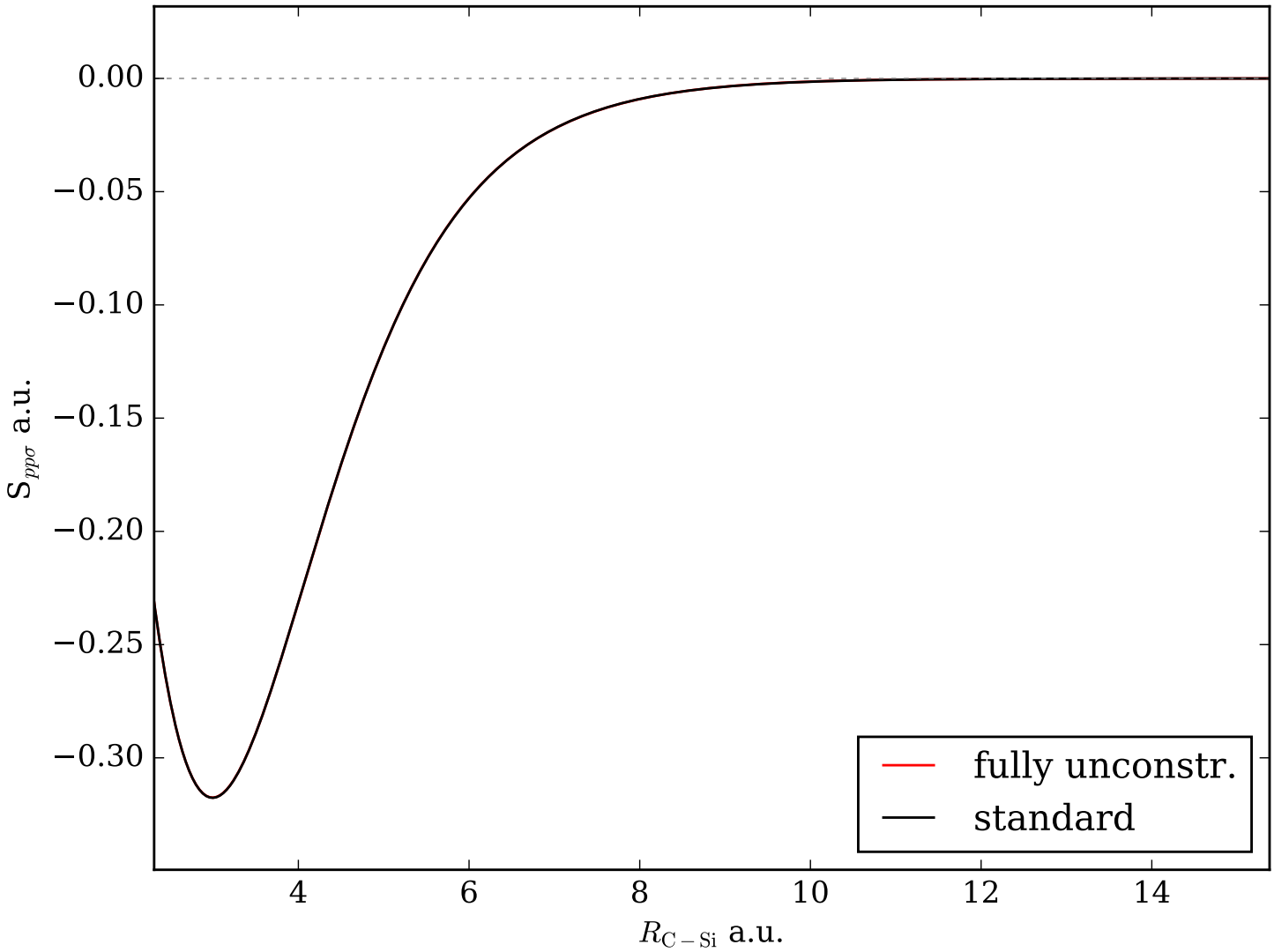
10
12
14
$R_{\mathrm{C-Si}}$ a.u.
fully unconstr.
standard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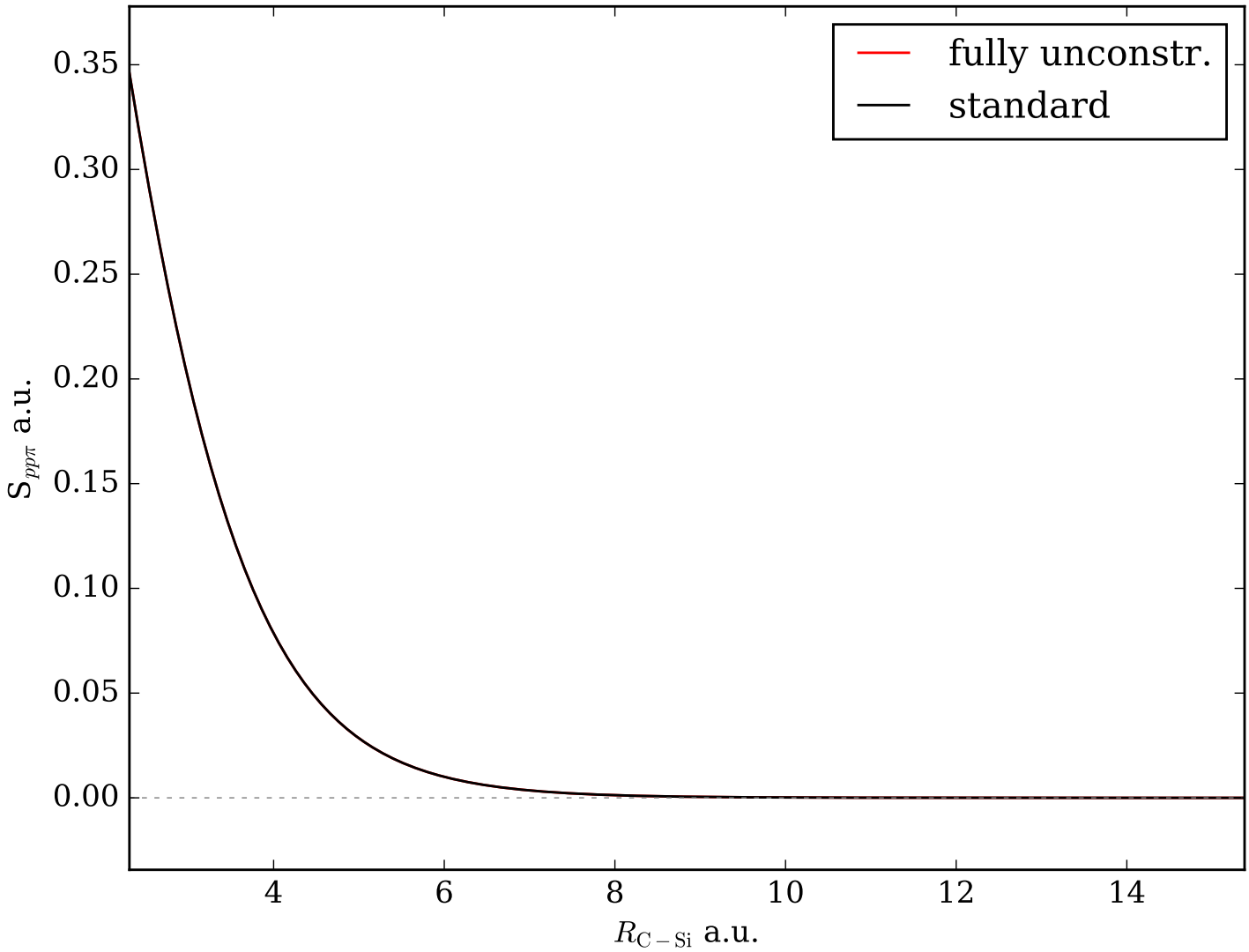
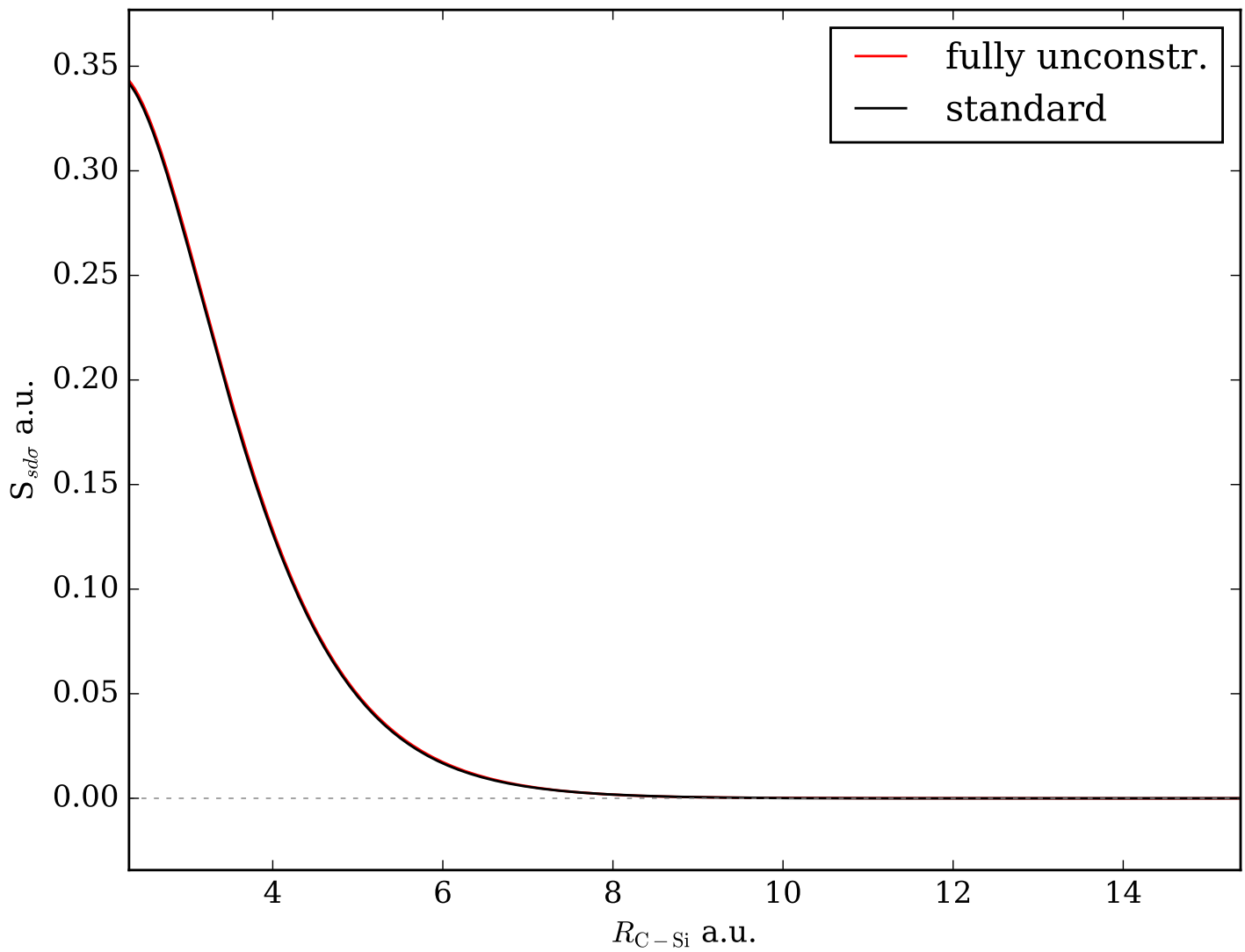
−0.25
−0.30
$S_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Si}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$S_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Si}}$ a.u.


fully unconstr.
standard
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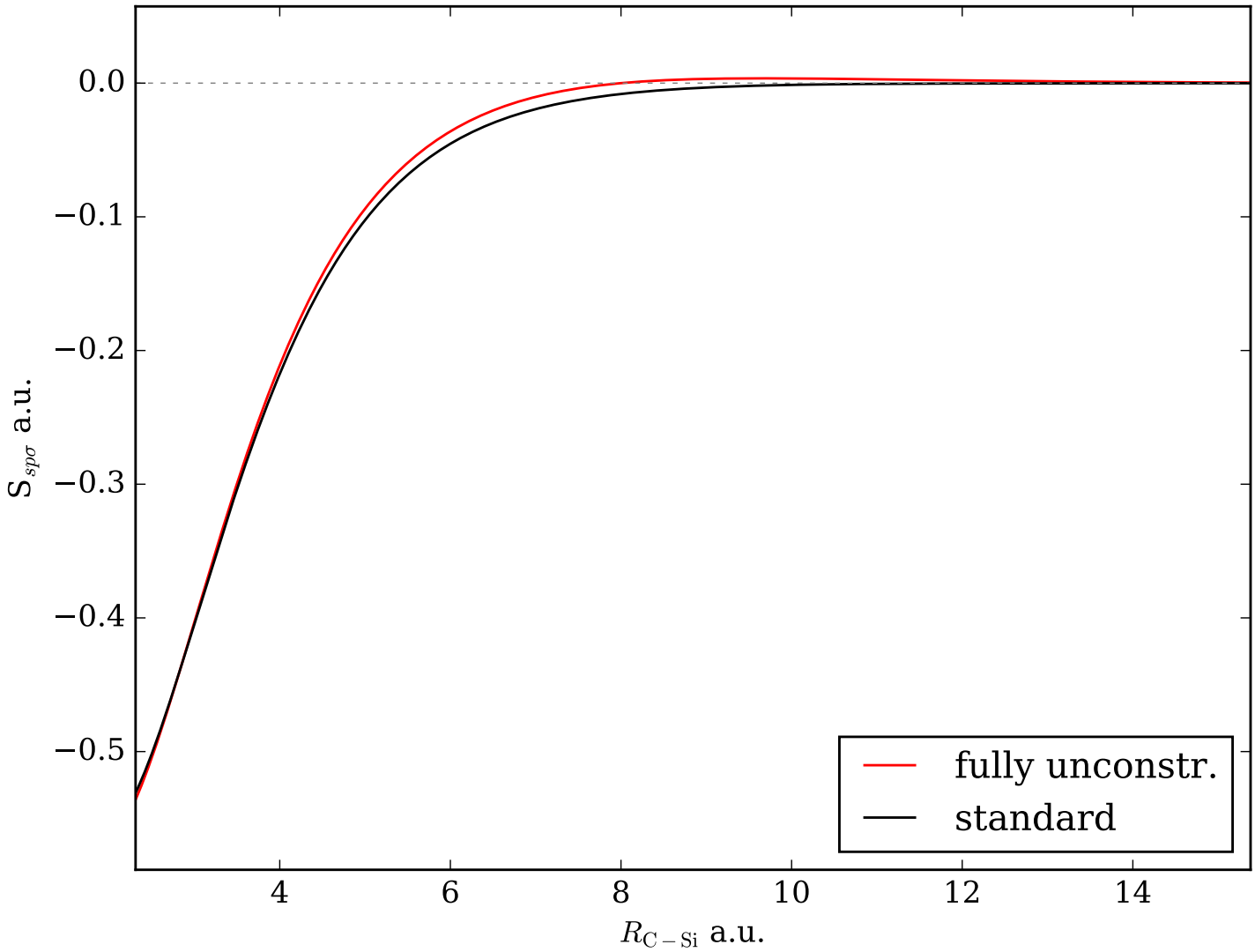
0.20
0.15
0.10
0.05
0.00
$S_{sd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Si}}$ a.u.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−0.2
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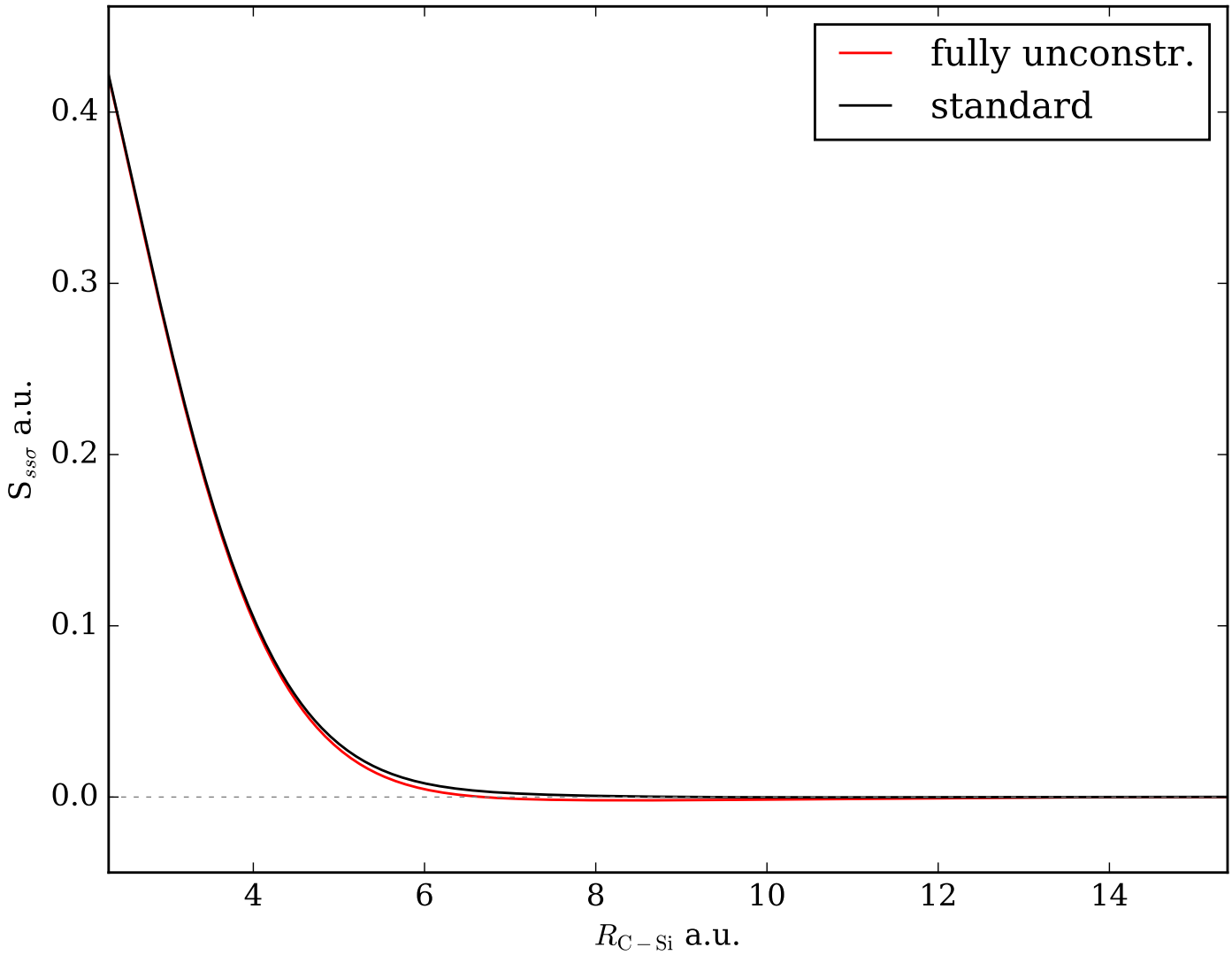
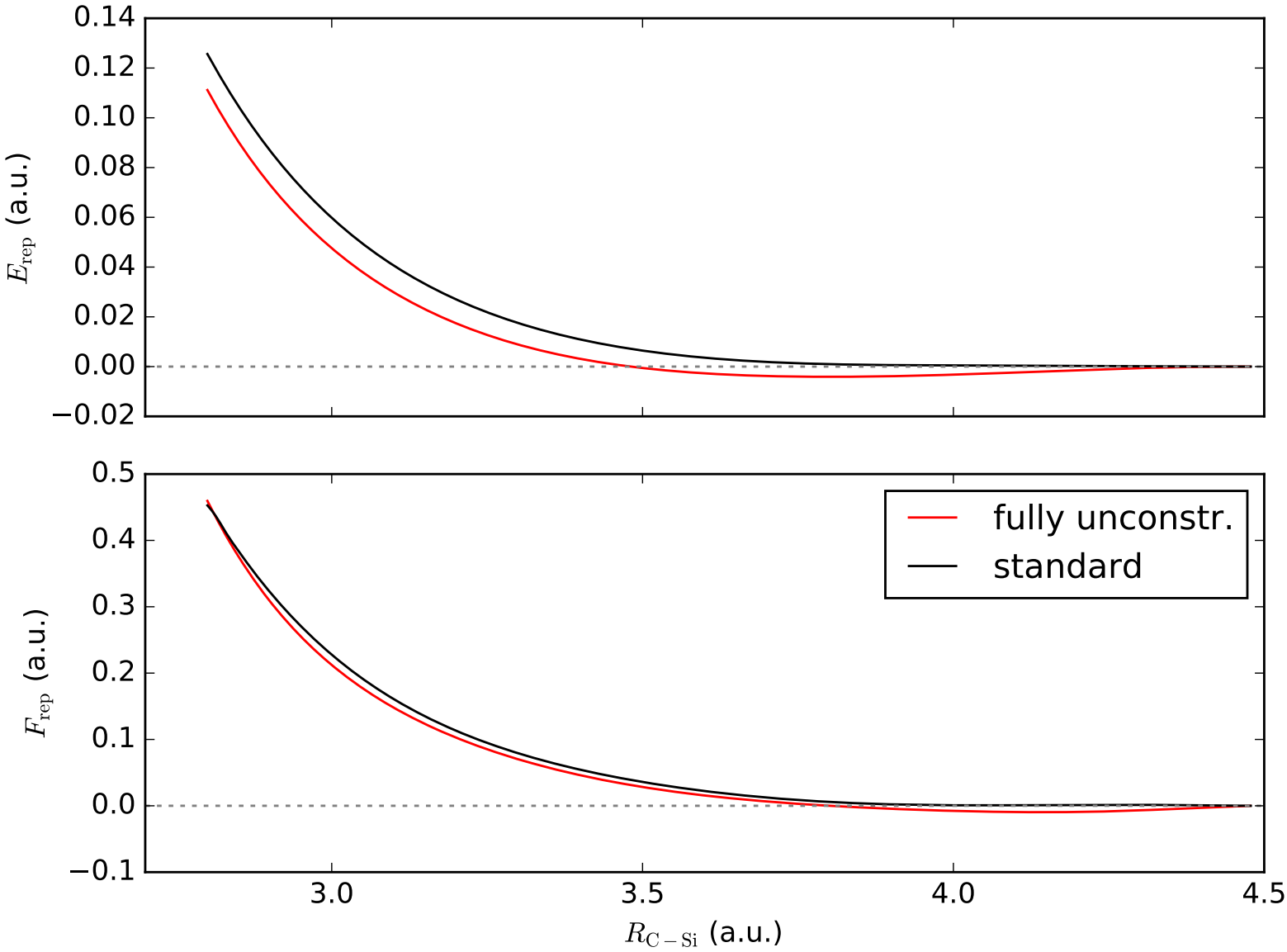
−0.4
−0.5
$S_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Si}}$ a.u.
fully unconstr.
standard

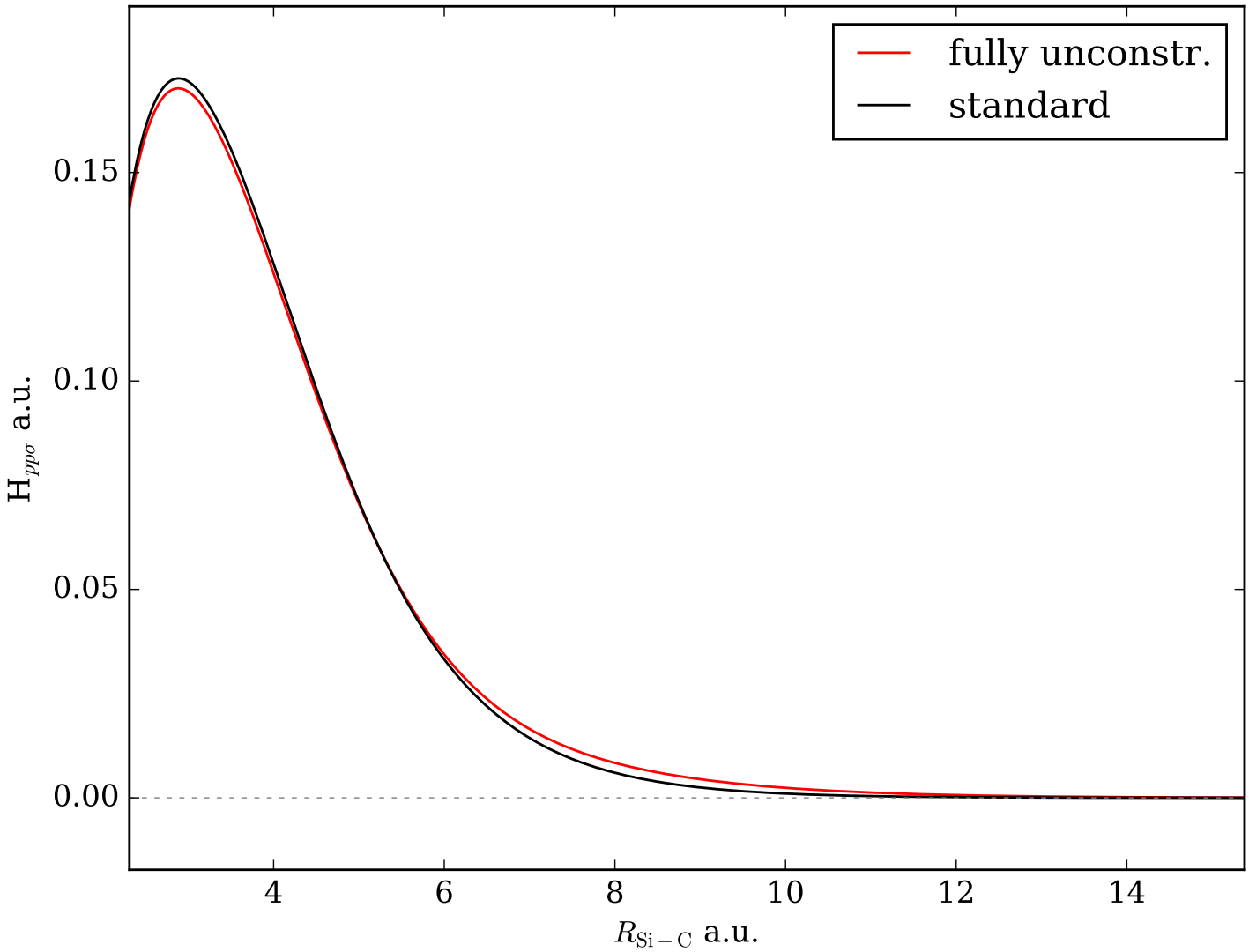

fully unconstr.
standard
0.4
0.3
0.2
0.1
0.0
$S_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Si}}$ a.u.

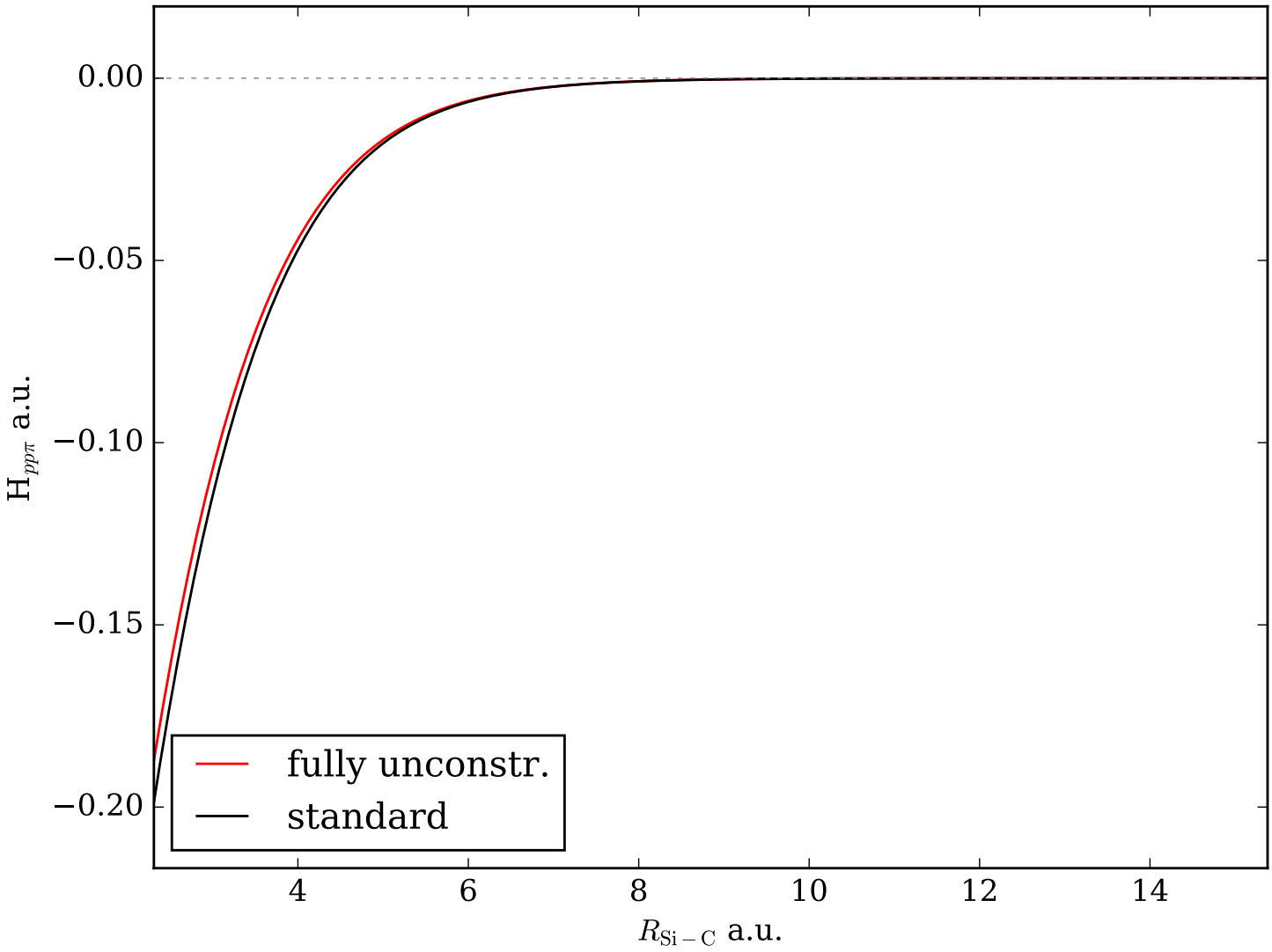
5.2 Repulsive

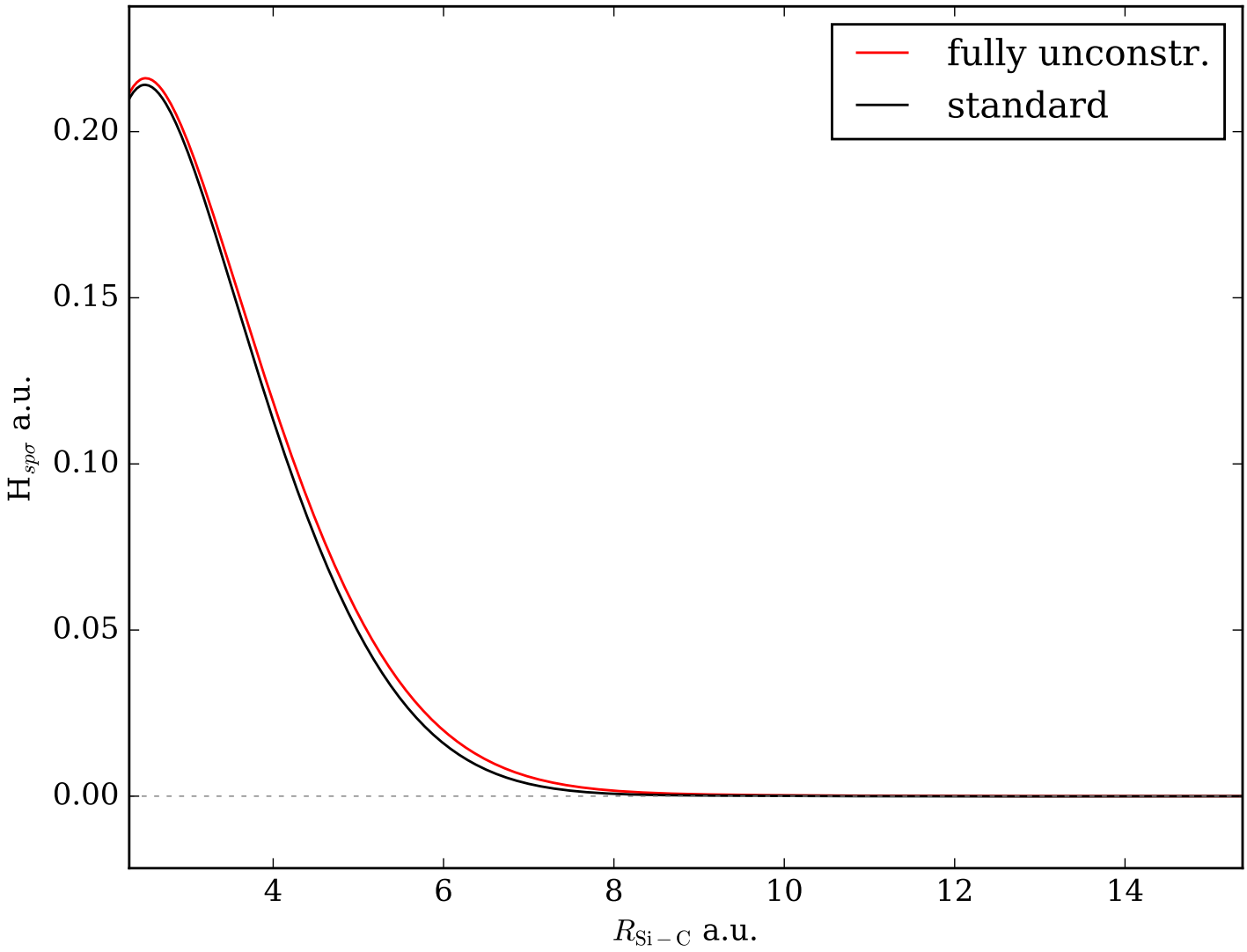


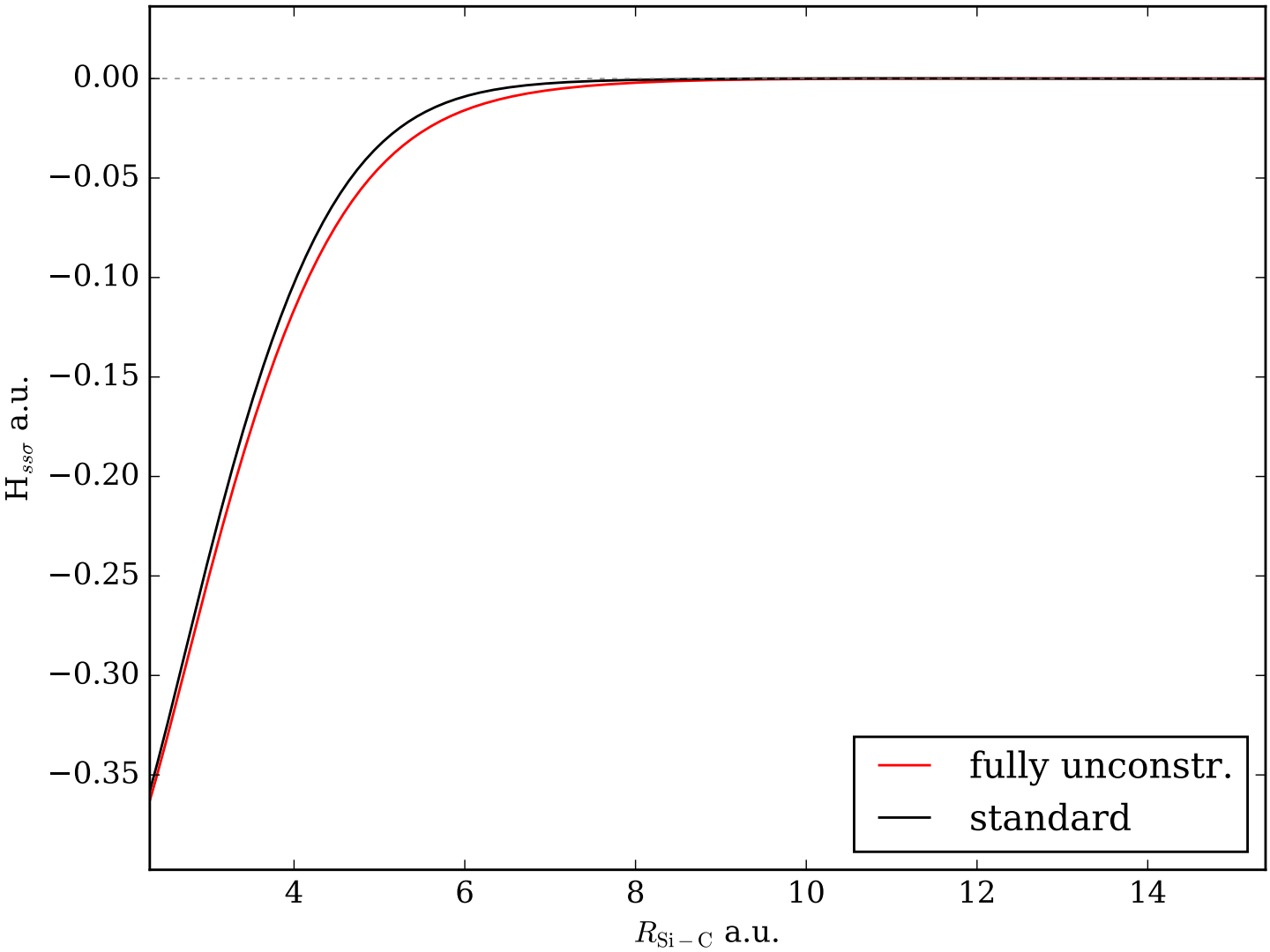
6 Si-C

6.1 Electronic




0.00
−0.05
−0.10
−0.15
−0.20
$H_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-C}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.20
0.15
0.10
0.05
0.00
$H_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-C}}$ a.u.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−0.15
−0.20
−0.25
−0.30
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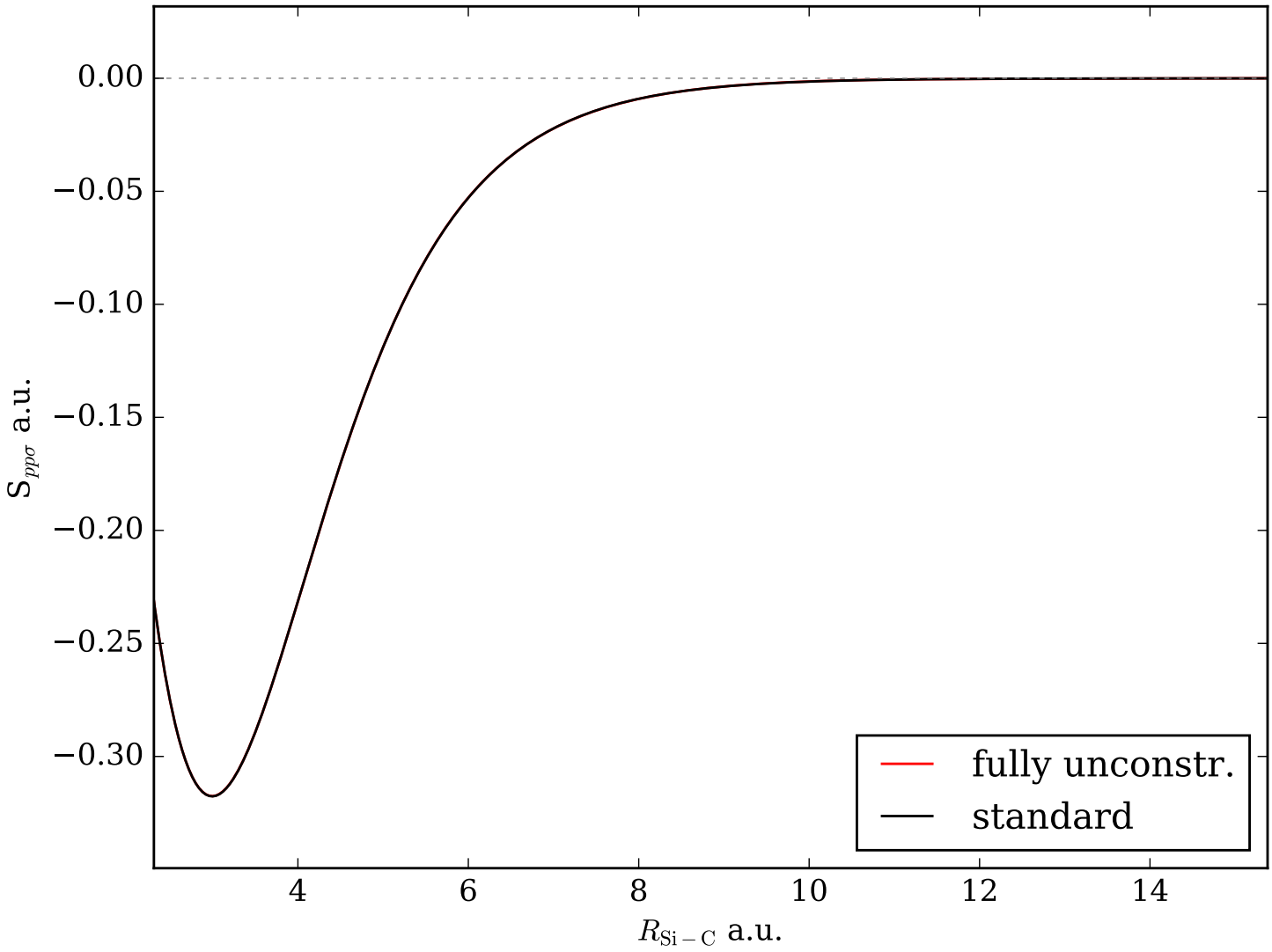
$H_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-C}}$ a.u.
fully unconstr.
standard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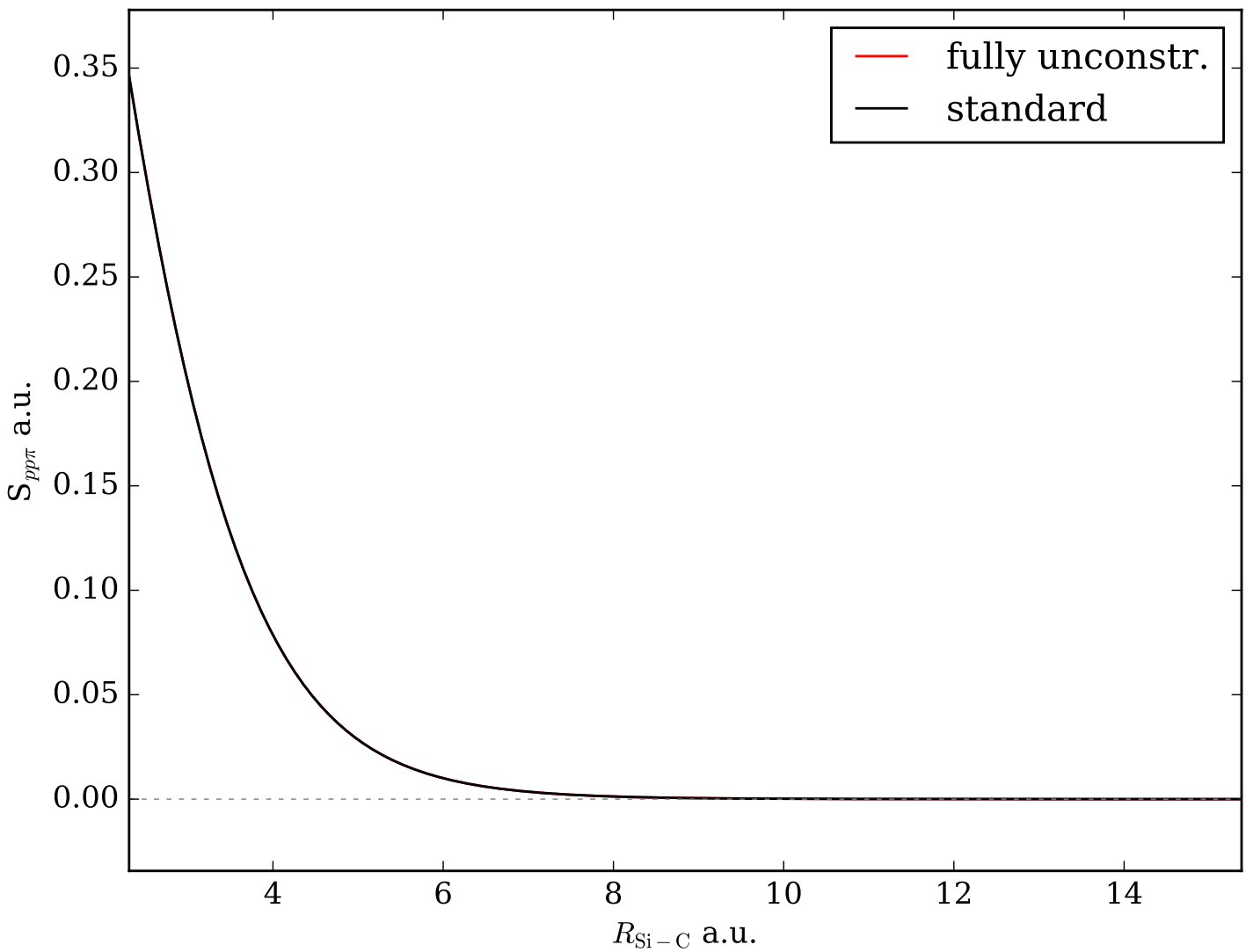
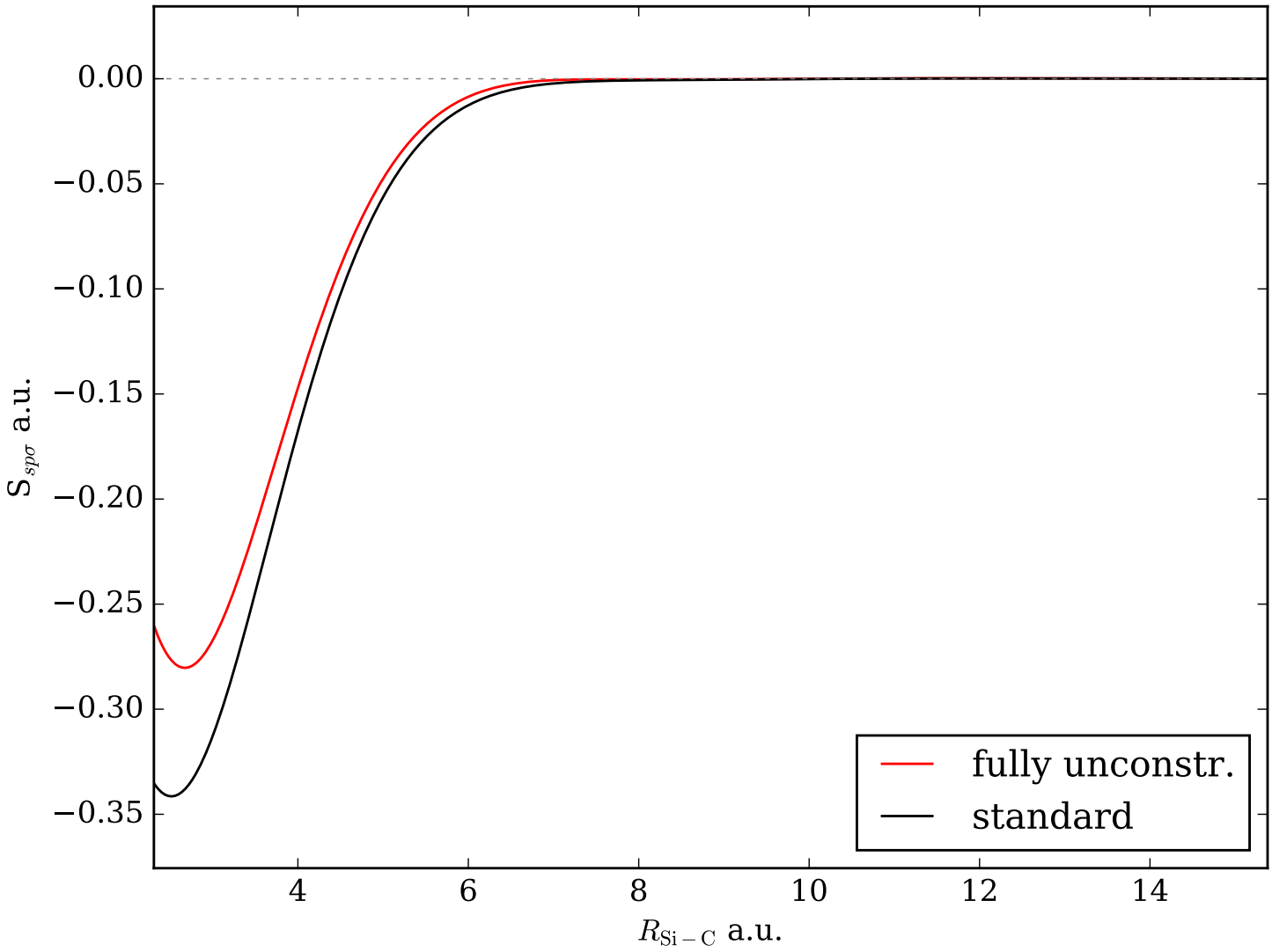
−0.20
−0.25
−0.30
$S_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-C}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$S_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-C}}$ a.u.


0.00
−0.05
−0.10
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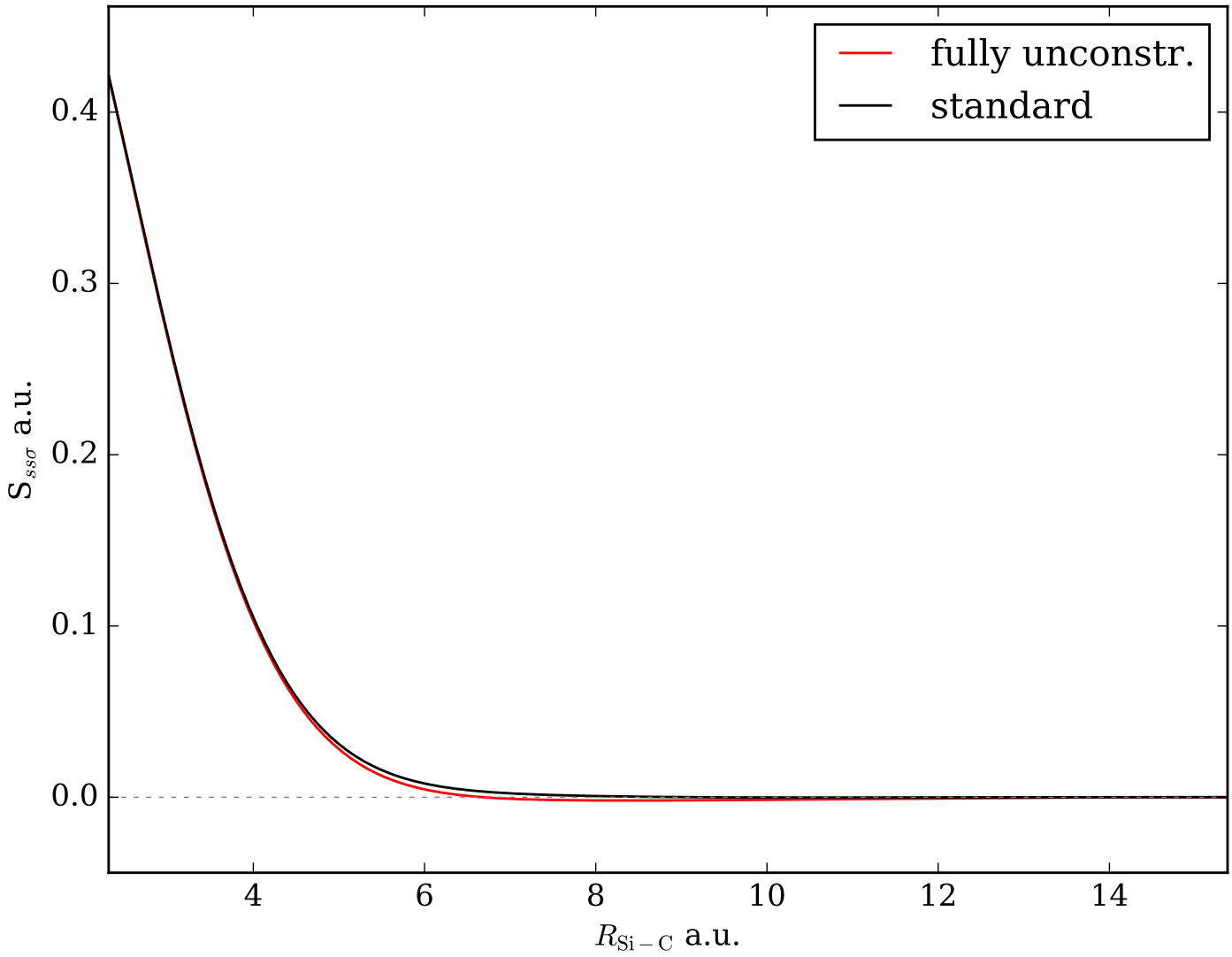
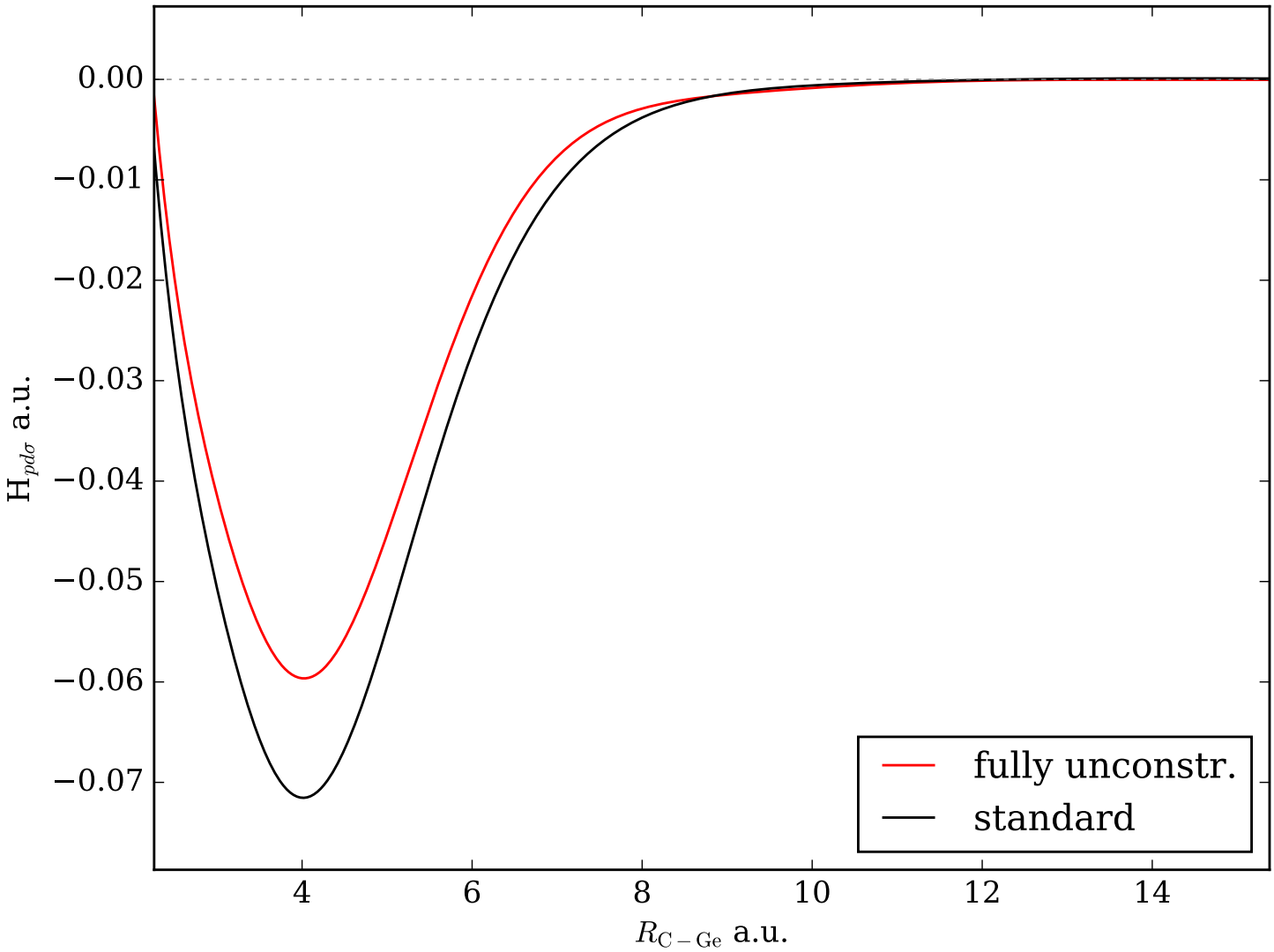
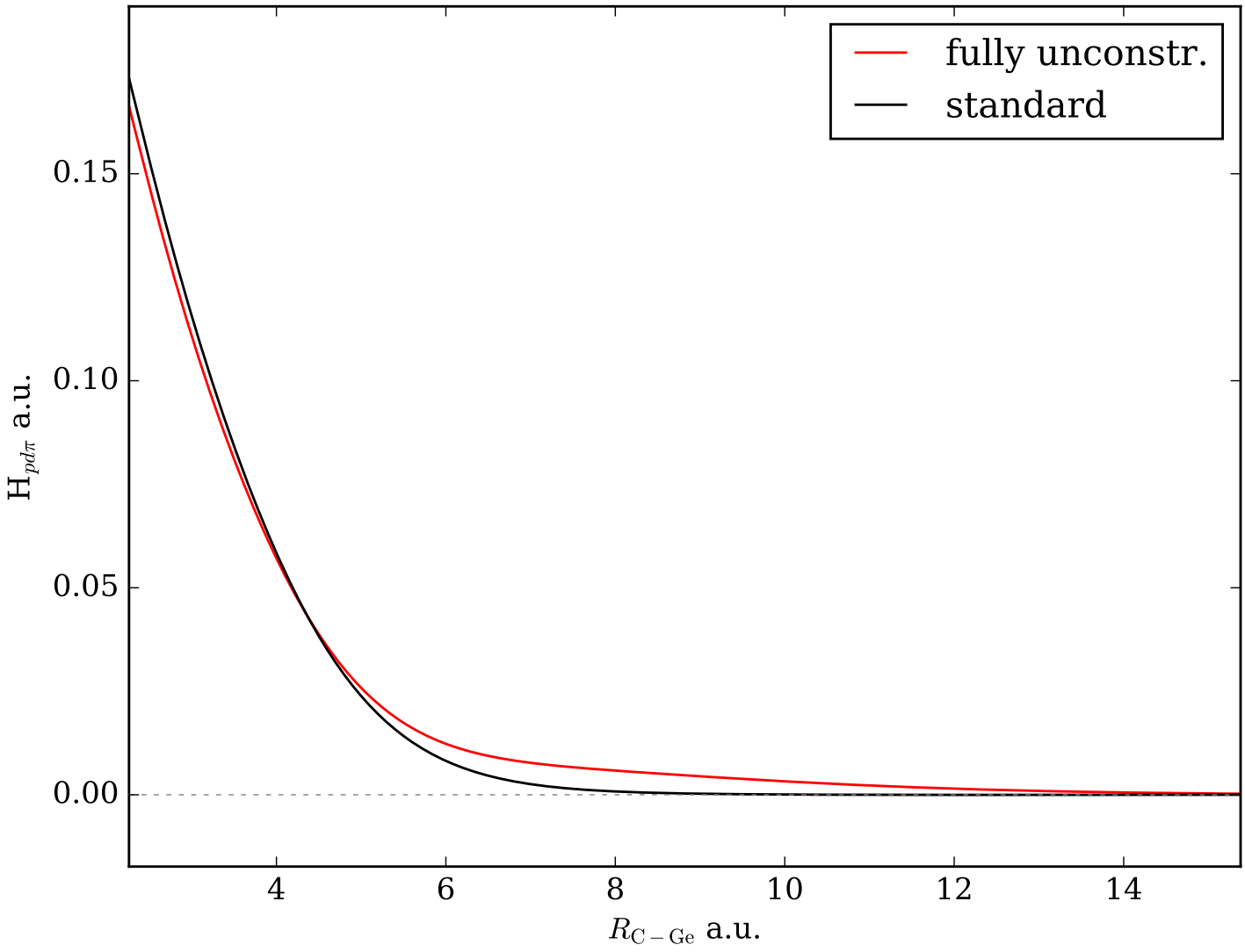
−0.20
−0.25
−0.30
−0.35
$S_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-C}}$ a.u.
fully unconstr.
standard

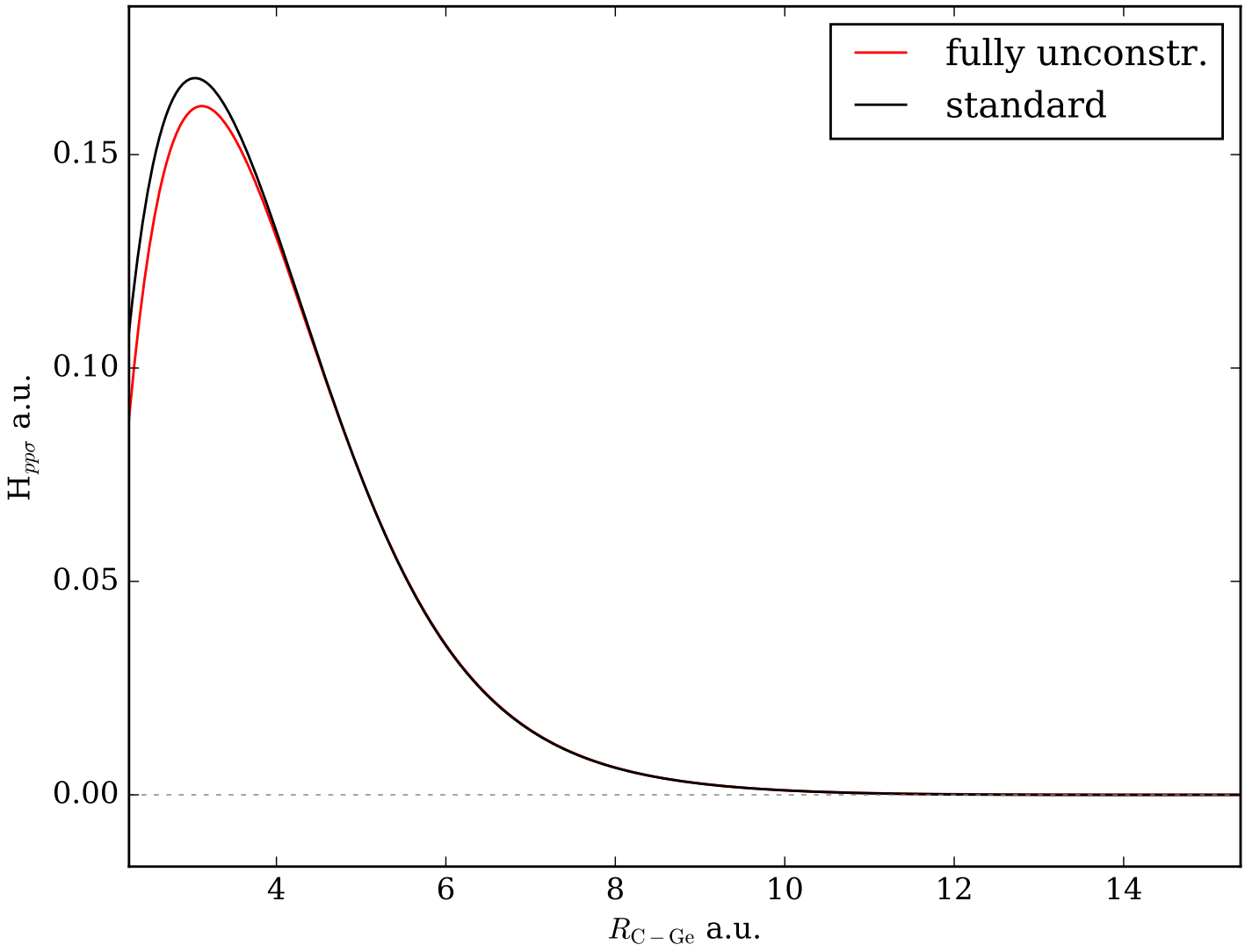

fully unconstr.
standard
0.4
0.3
0.2
0.1
0.0
$S_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-C}}$ a.u.

7 C-Ge

7.1 Electronic




fully unconstr.
standard
0.15
0.10
0.05
0.00
$H_{pd\pi}$ a.u.
4
6
8
10
12
14
R_{C-Ge} a.u.


fully unconstr.
standard
0.15
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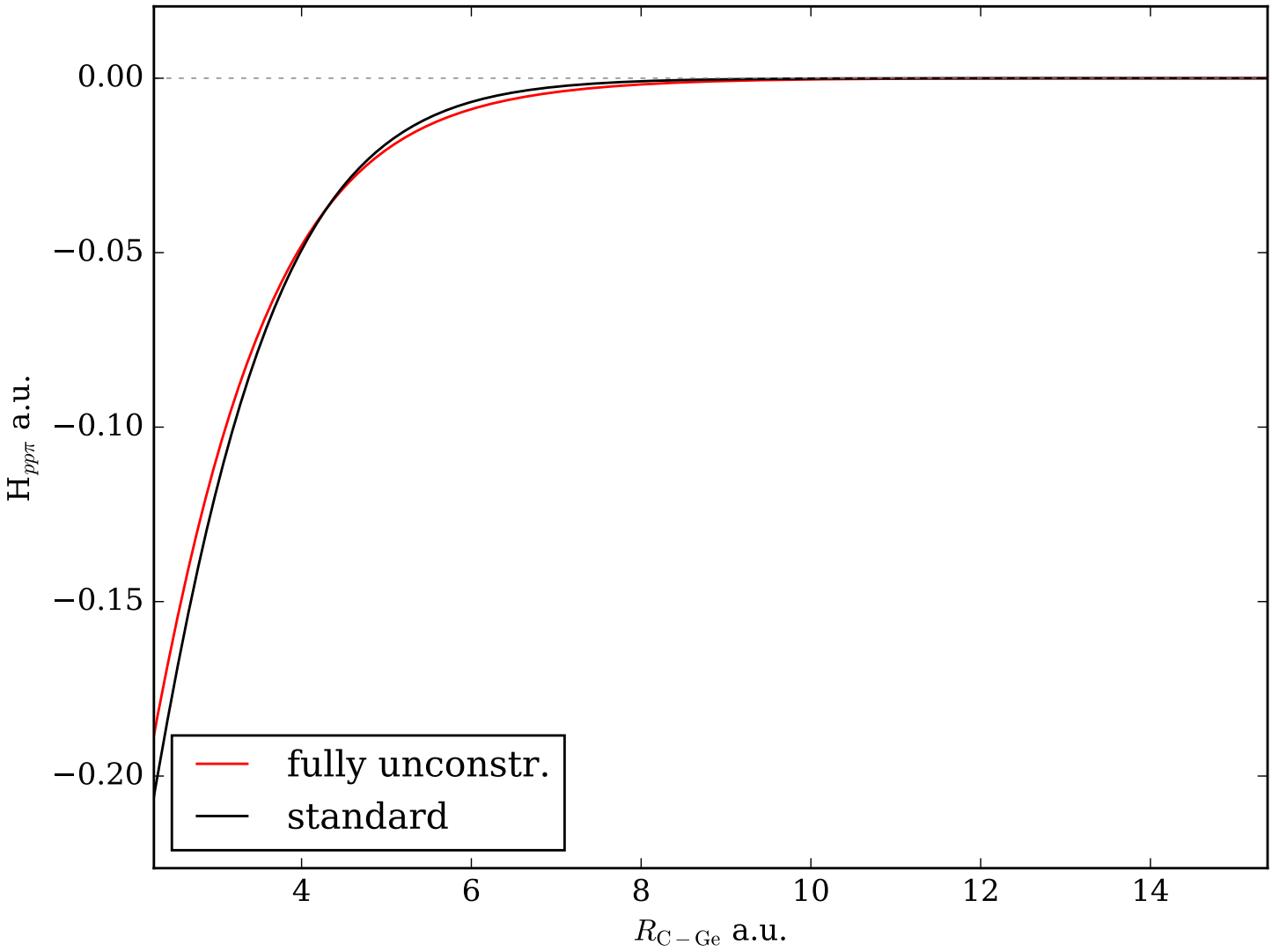
0.05
0.00
$H_{pp\sigma}$ a.u.
4
6
8
10
12
14
R_{C-Ge} a.u.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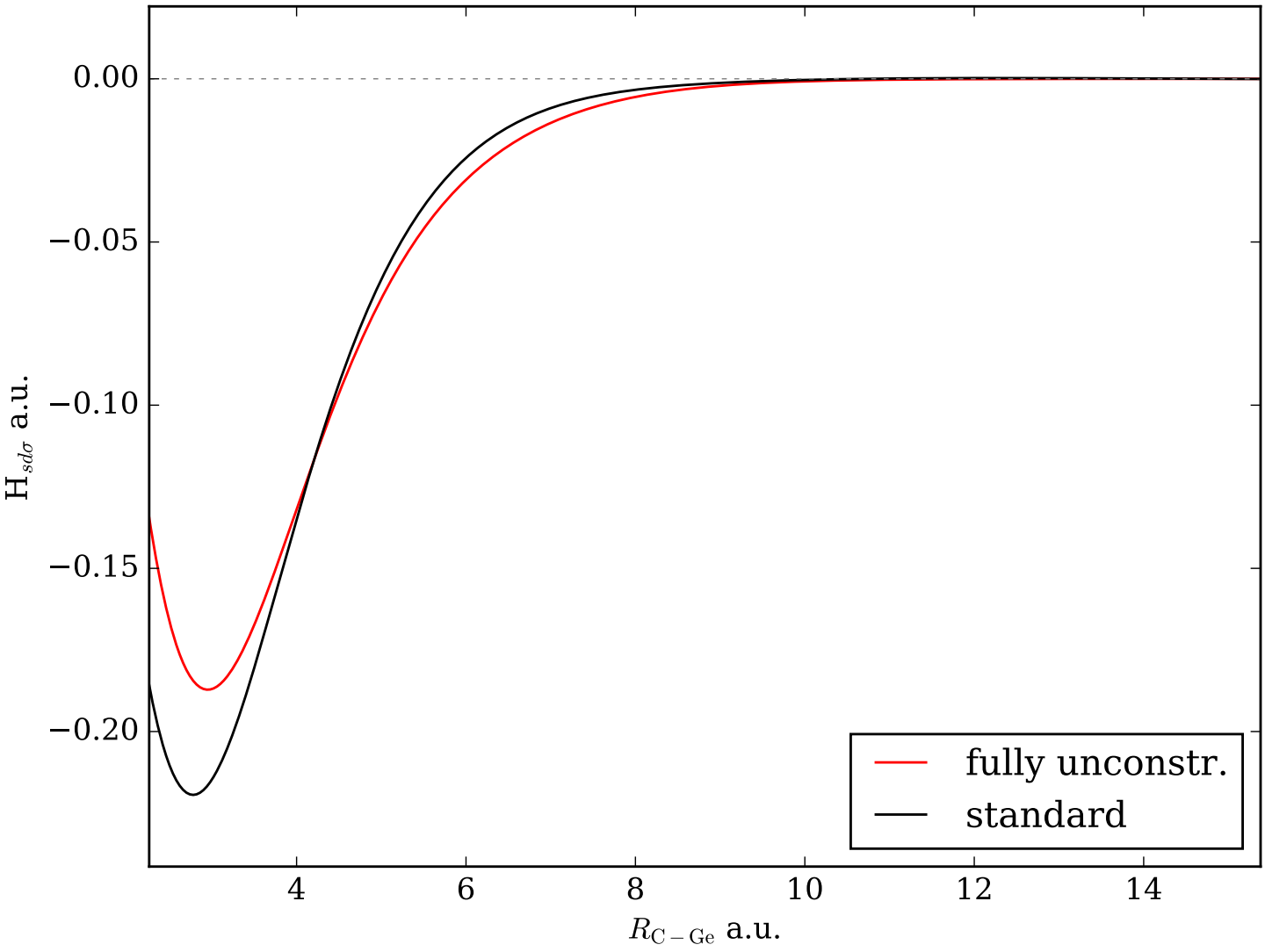
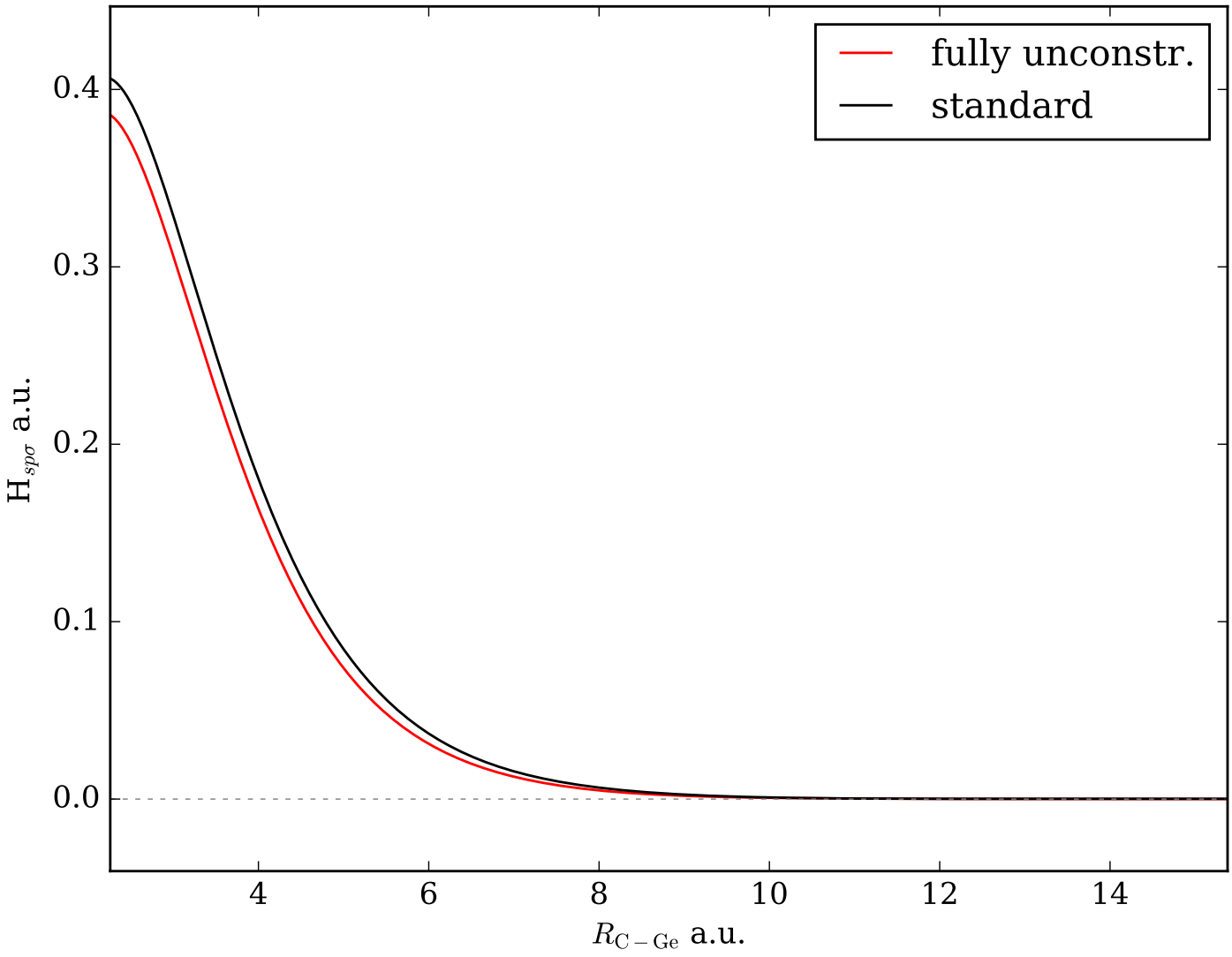
4
6
8
10
12
14
R_{C-Ge} a.u.
fully unconstr.
standard


0.00
−0.05
−0.10
−0.15
−0.20
$H_{sd\sigma}$ a.u.
4
6
8
10
12
14
R_{C-Ge} a.u.
fully unconstr.
standard


fully unconstr.
standard
0.4
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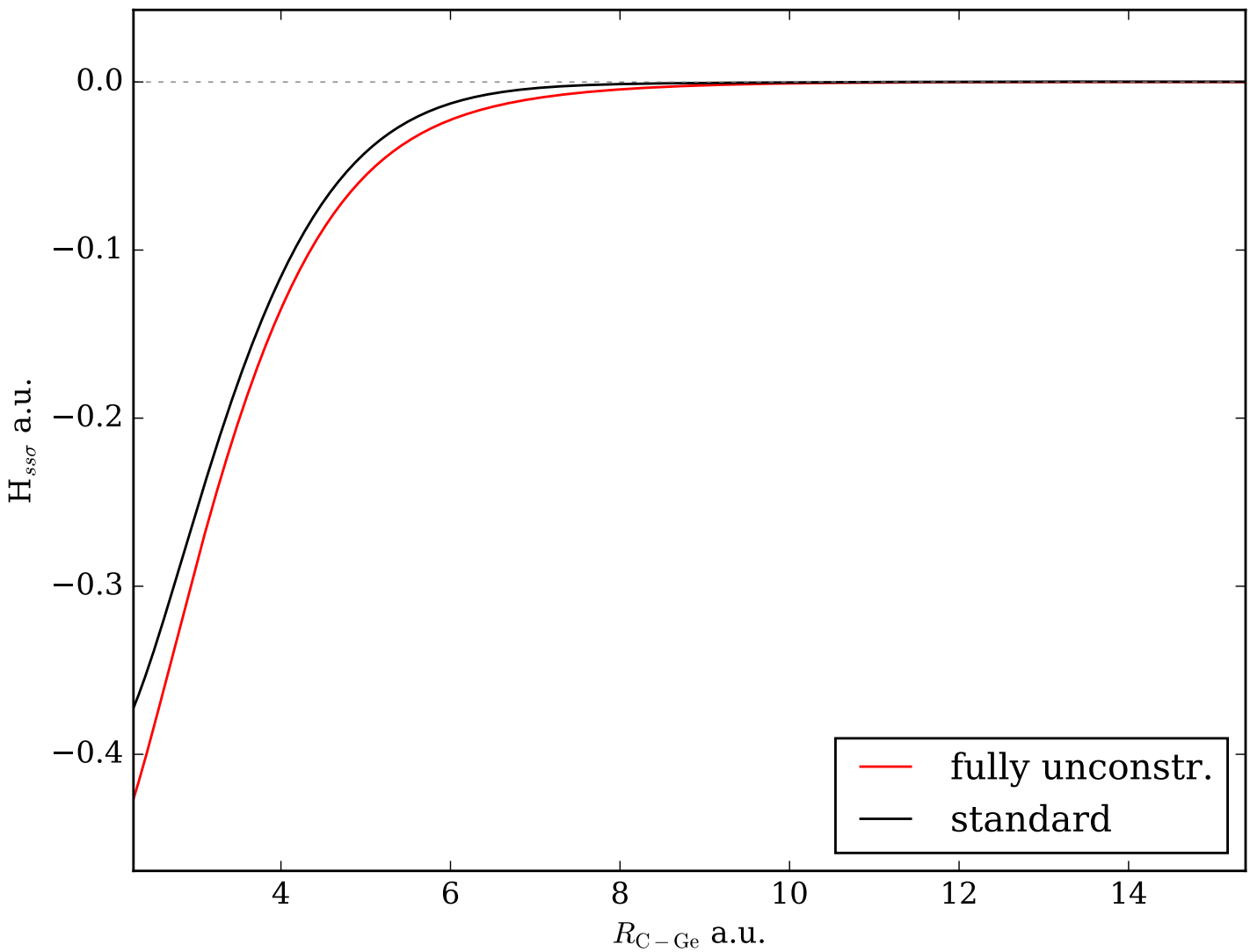
0.2
0.1
0.0
$H_{sp\sigma}$ a.u.
4
6
8
10
12
14
R_{C-Ge} a.u.


0.0
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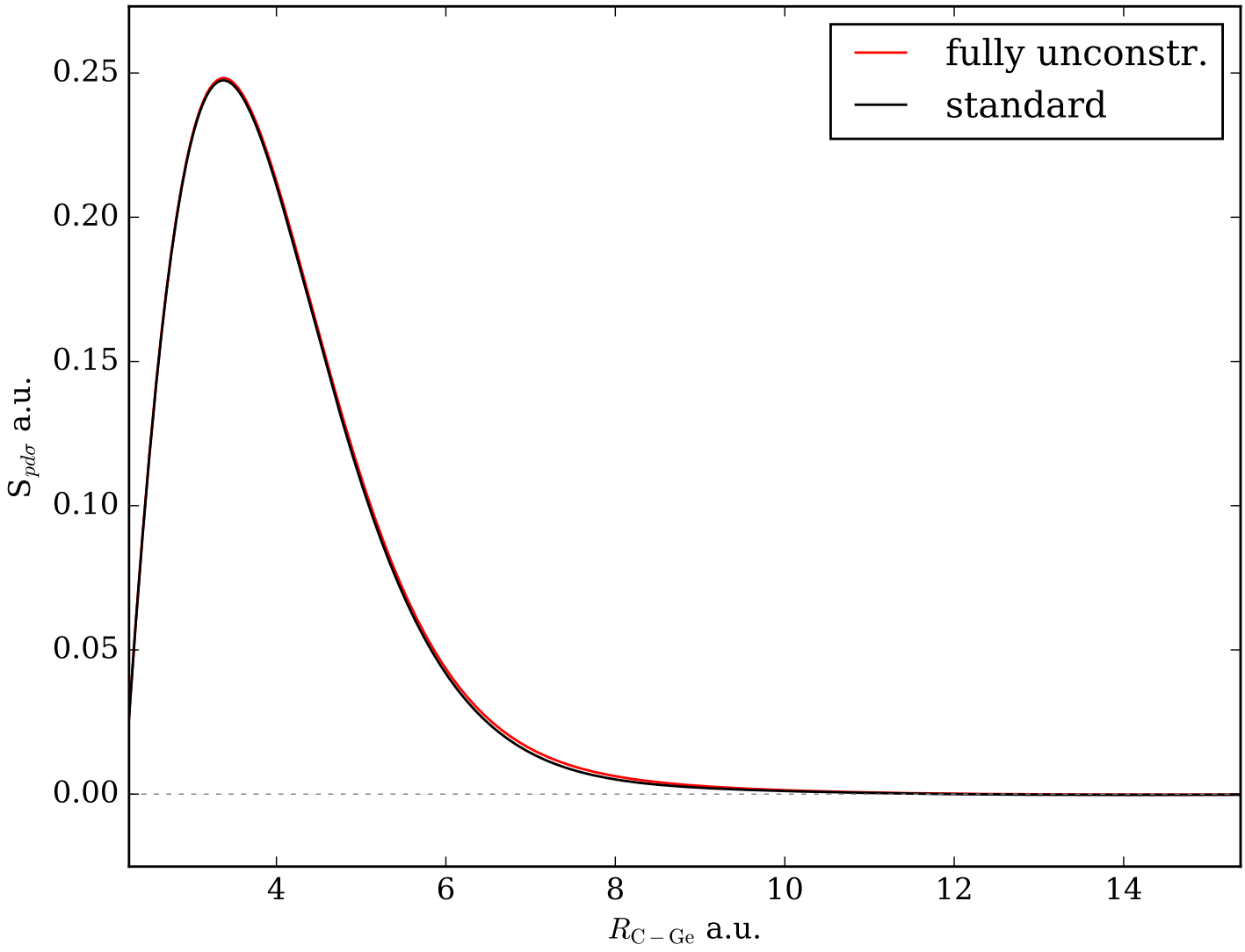
−0.2
−0.3
−0.4
$H_{ss\sigma}$ a.u.
4
6
8
10
12
14
R_{C-Ge} a.u.
fully unconstr.
standard


fully unconstr.
standard
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0.20
0.15
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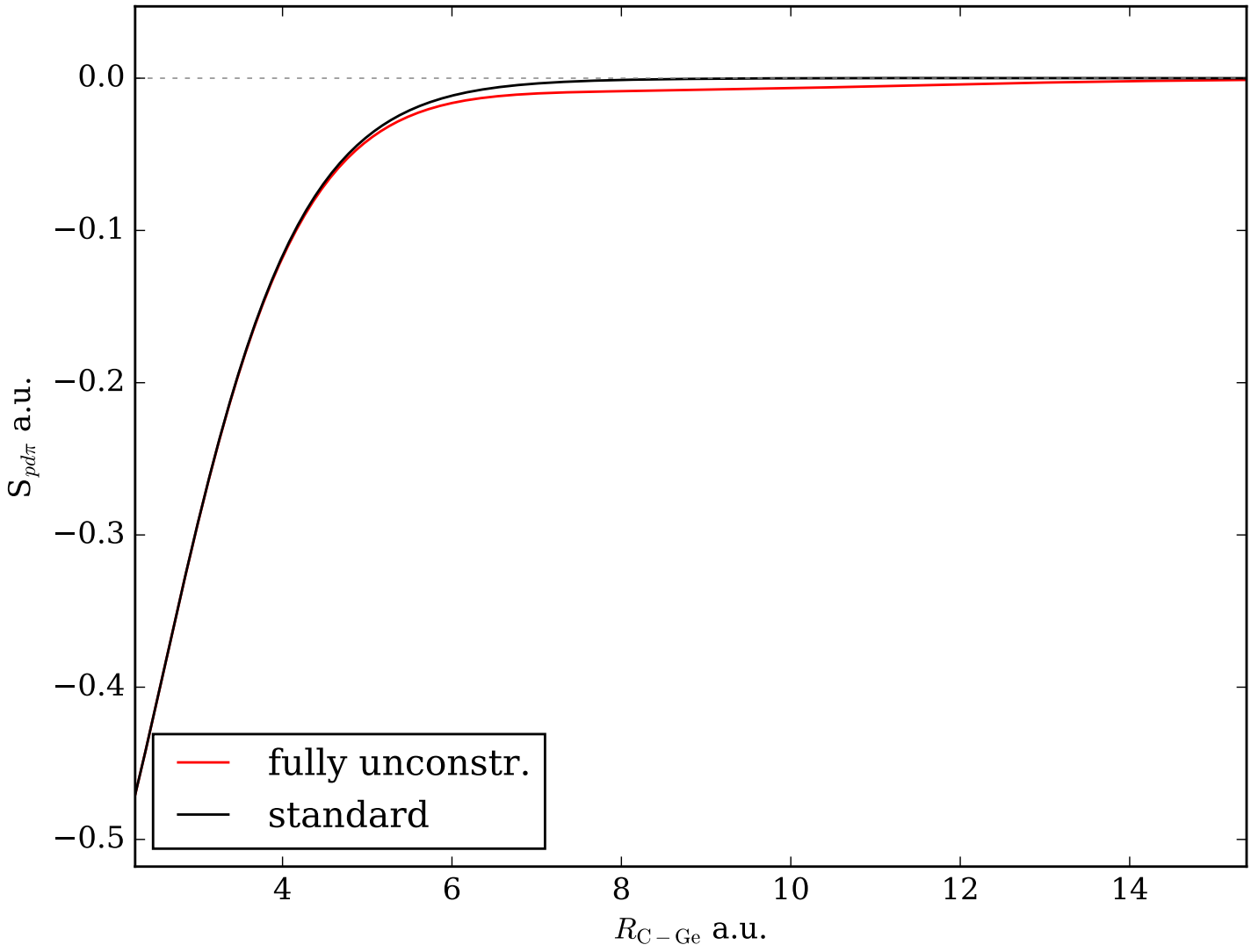
0.05
0.00
$S_{pd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Ge}}$ a.u.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−0.3
−0.4
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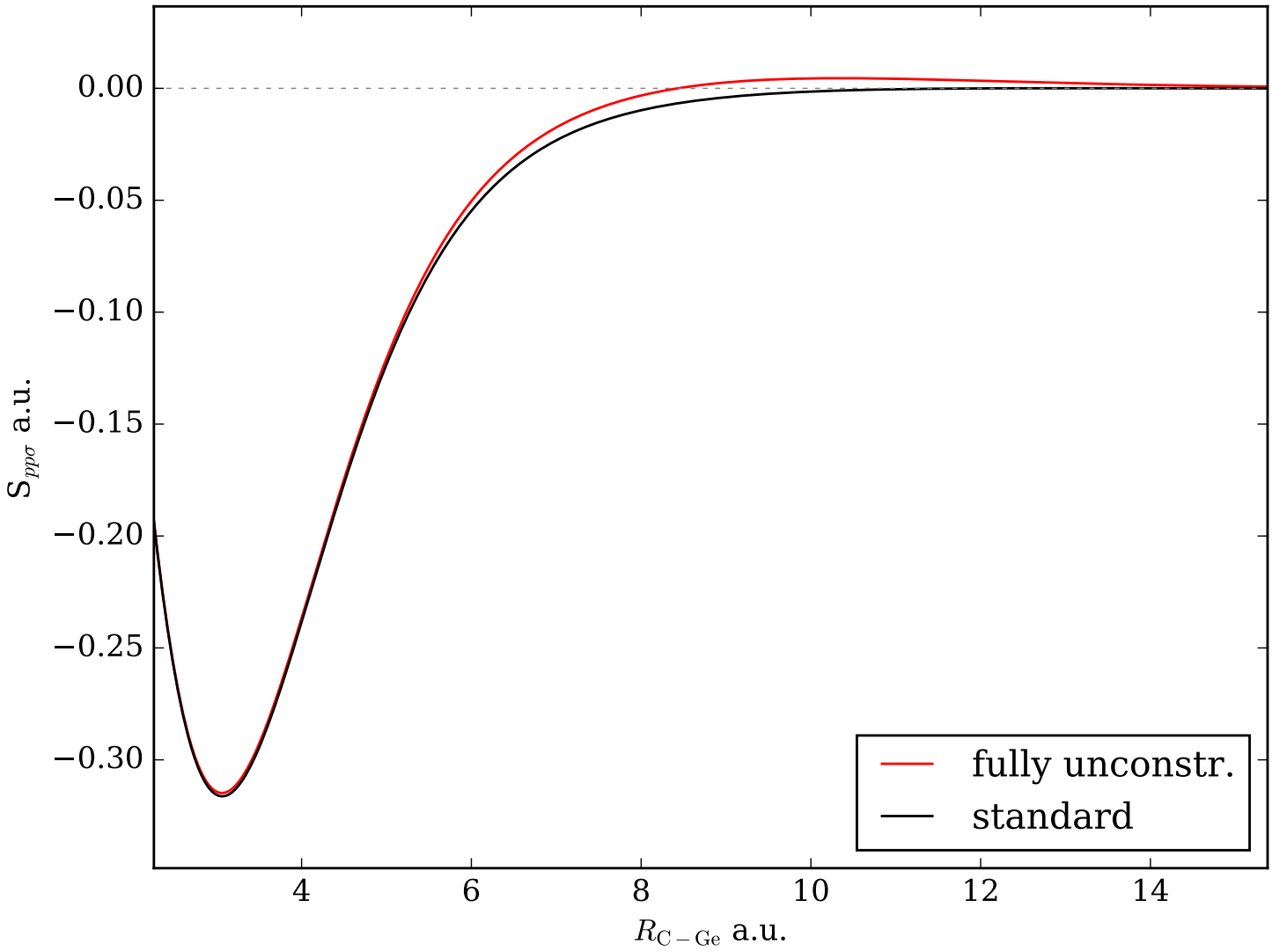
$S_{pd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Ge}}$ a.u.
fully unconstr.
standard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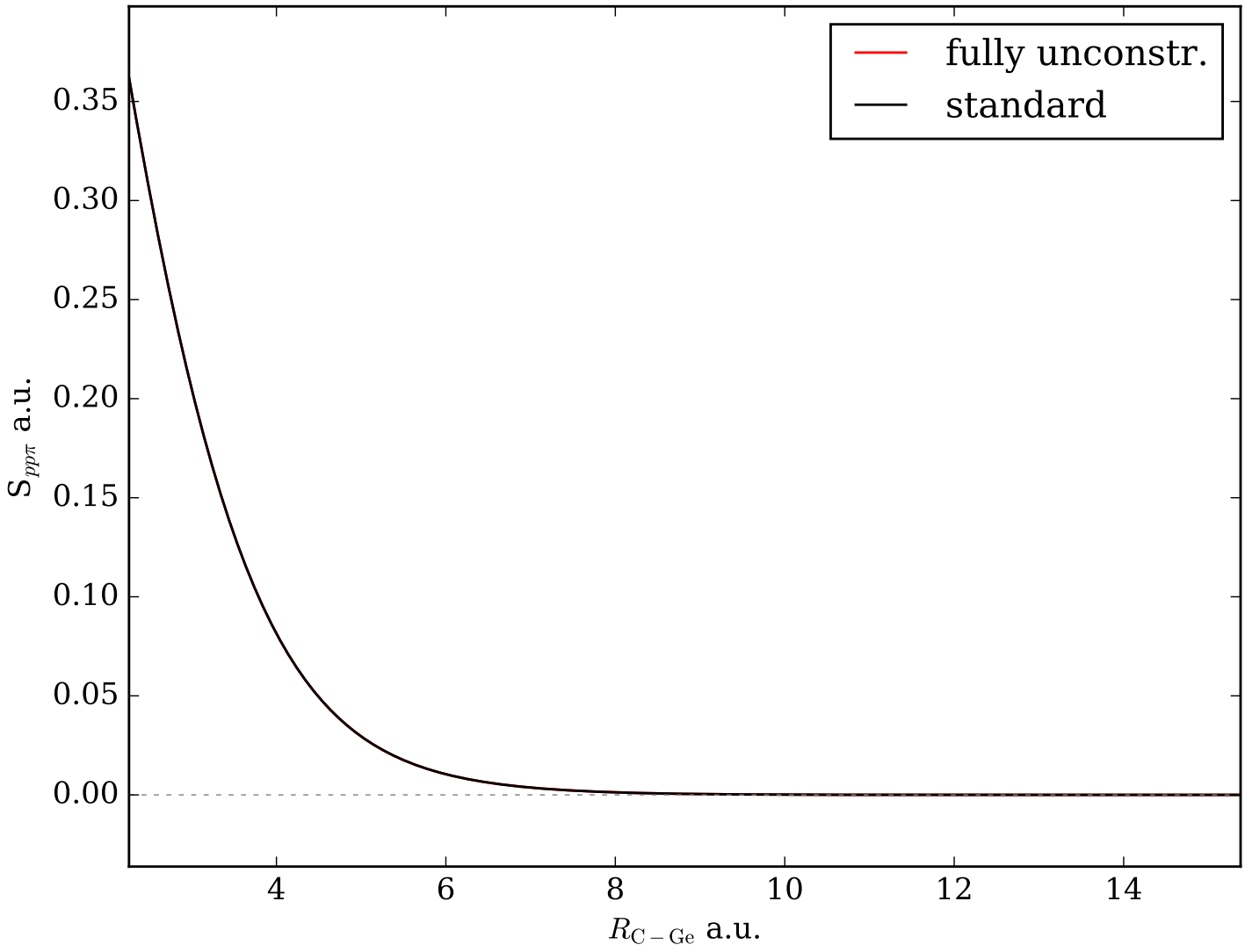
−0.20
−0.25
−0.30
$S_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Ge}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
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0.30
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0.20
0.15
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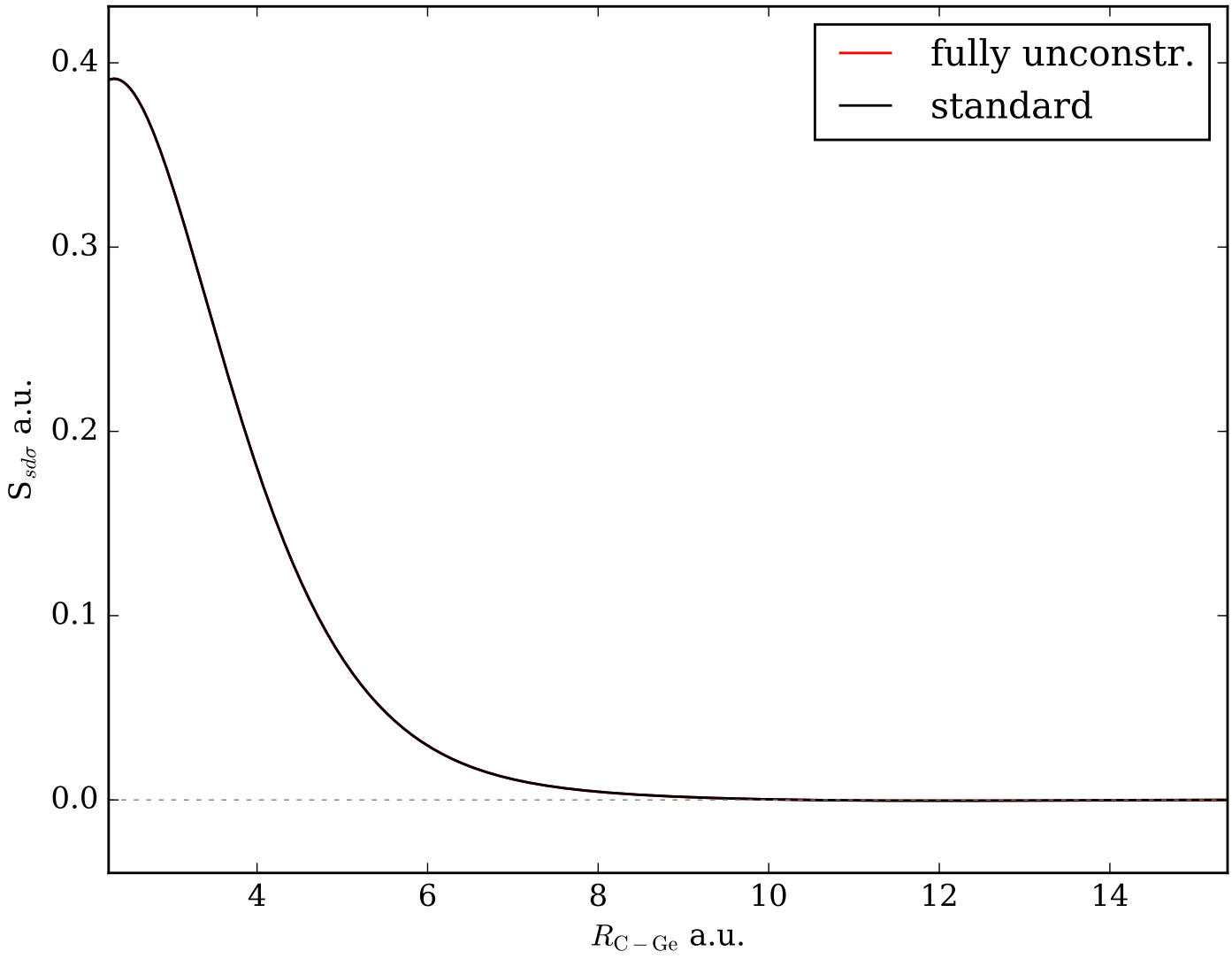
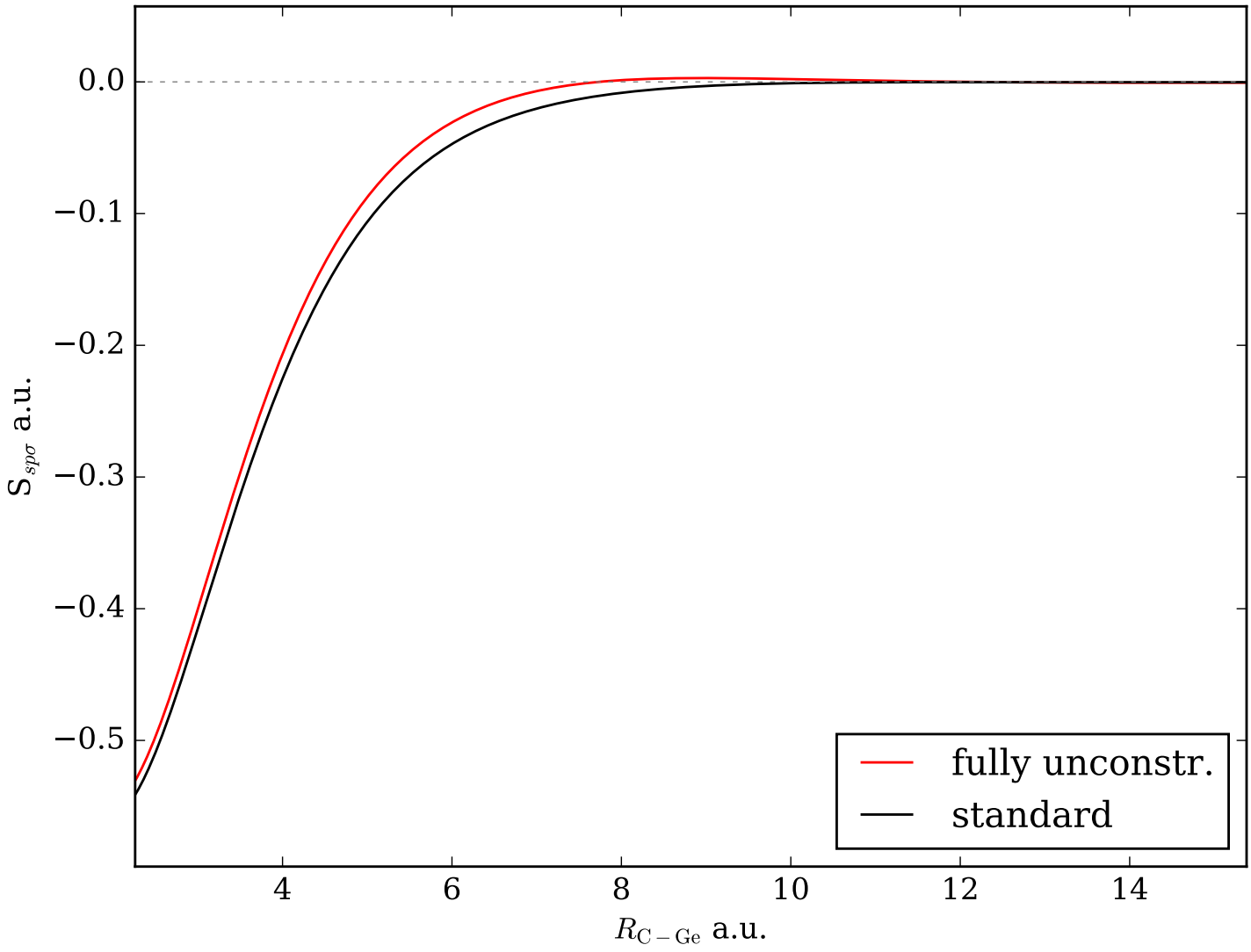
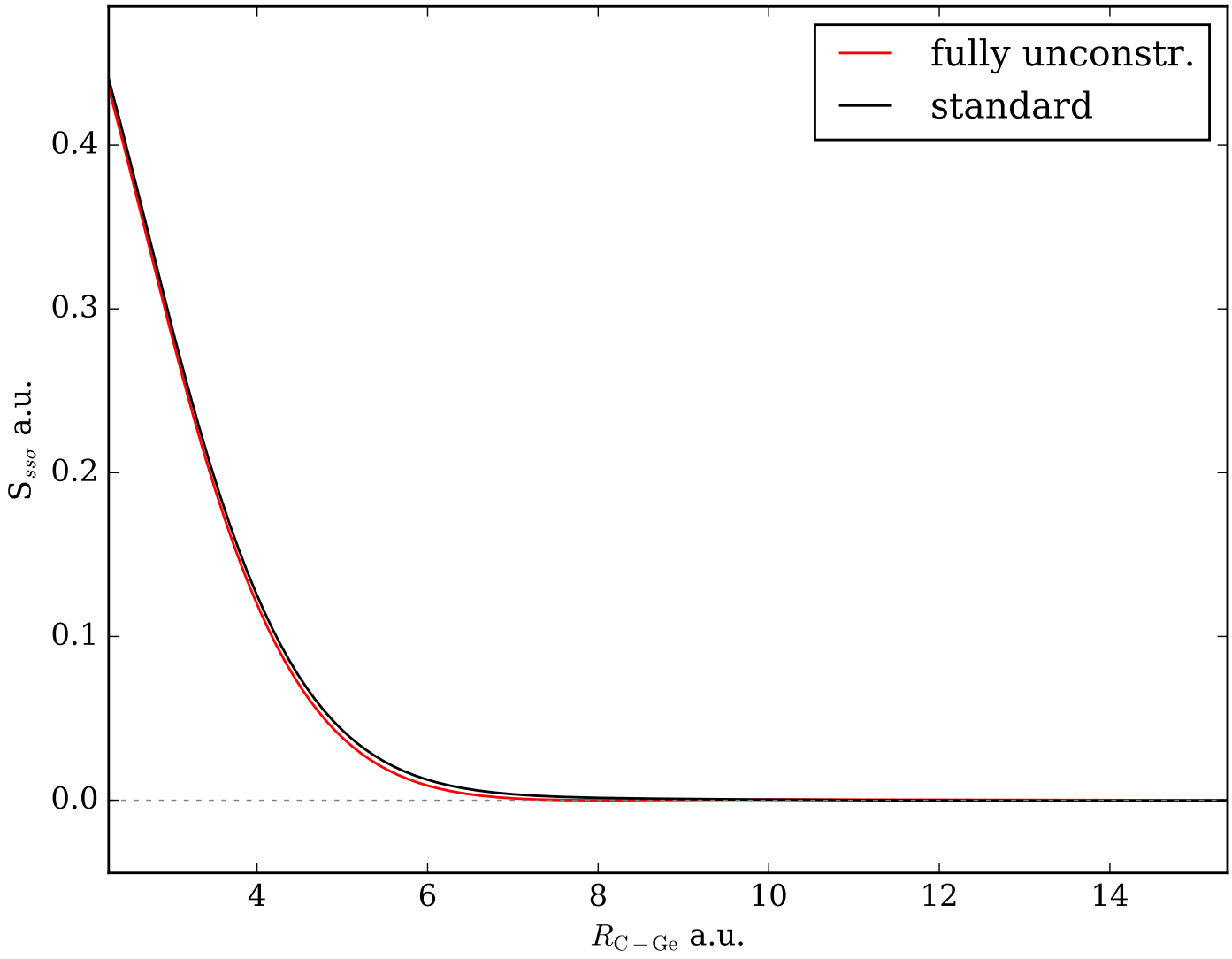
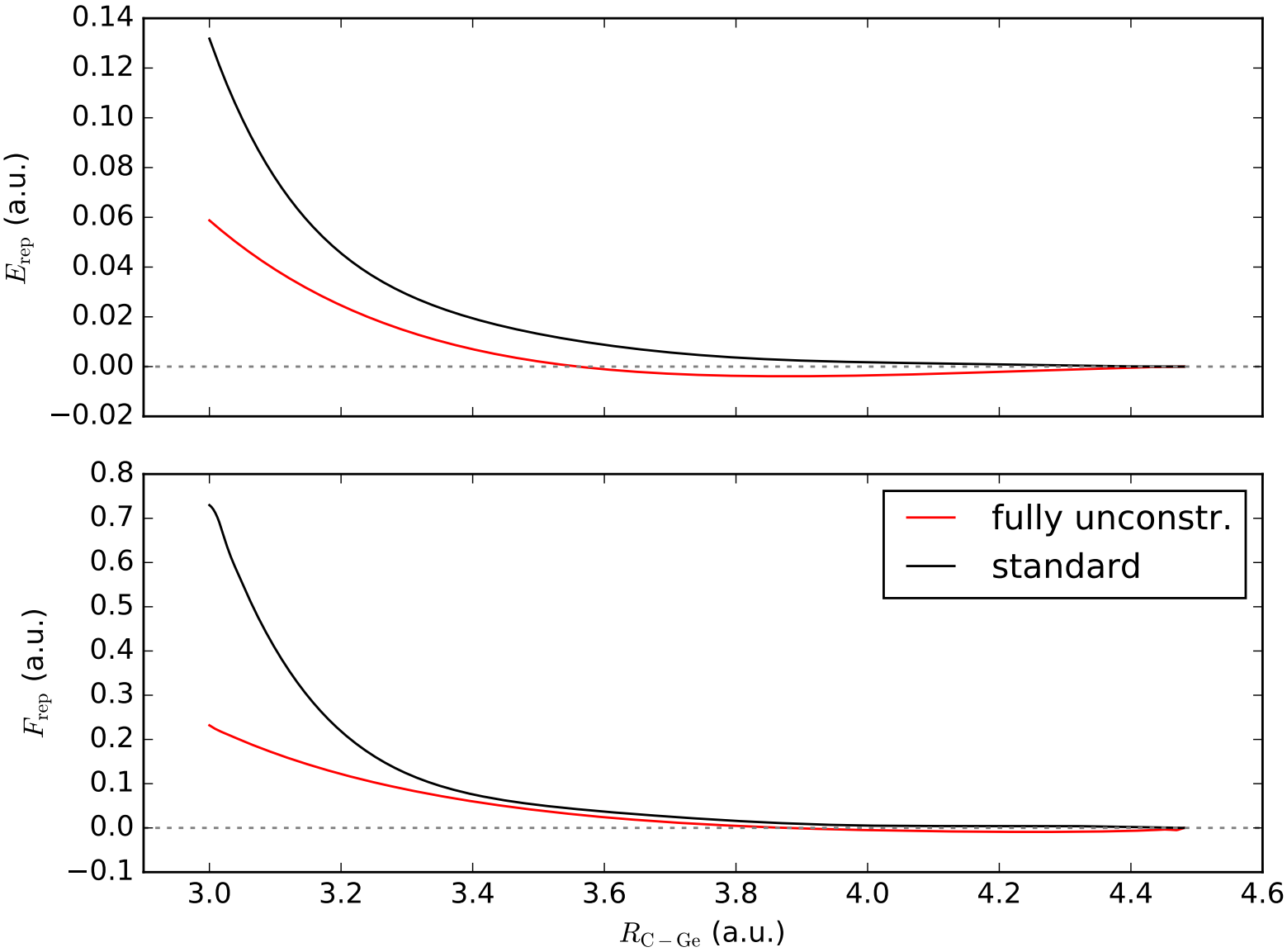
0.05
0.00
$S_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Ge}}$ a.u.


fully unconstr.
standard
0.4
0.3
0.2
0.1
0.0
$S_{sd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Ge}}$ a.u.


0.0
−0.1
−0.2
−0.3
−0.4
−0.5
$S_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Ge}}$ a.u.
fully unconstr.
standard

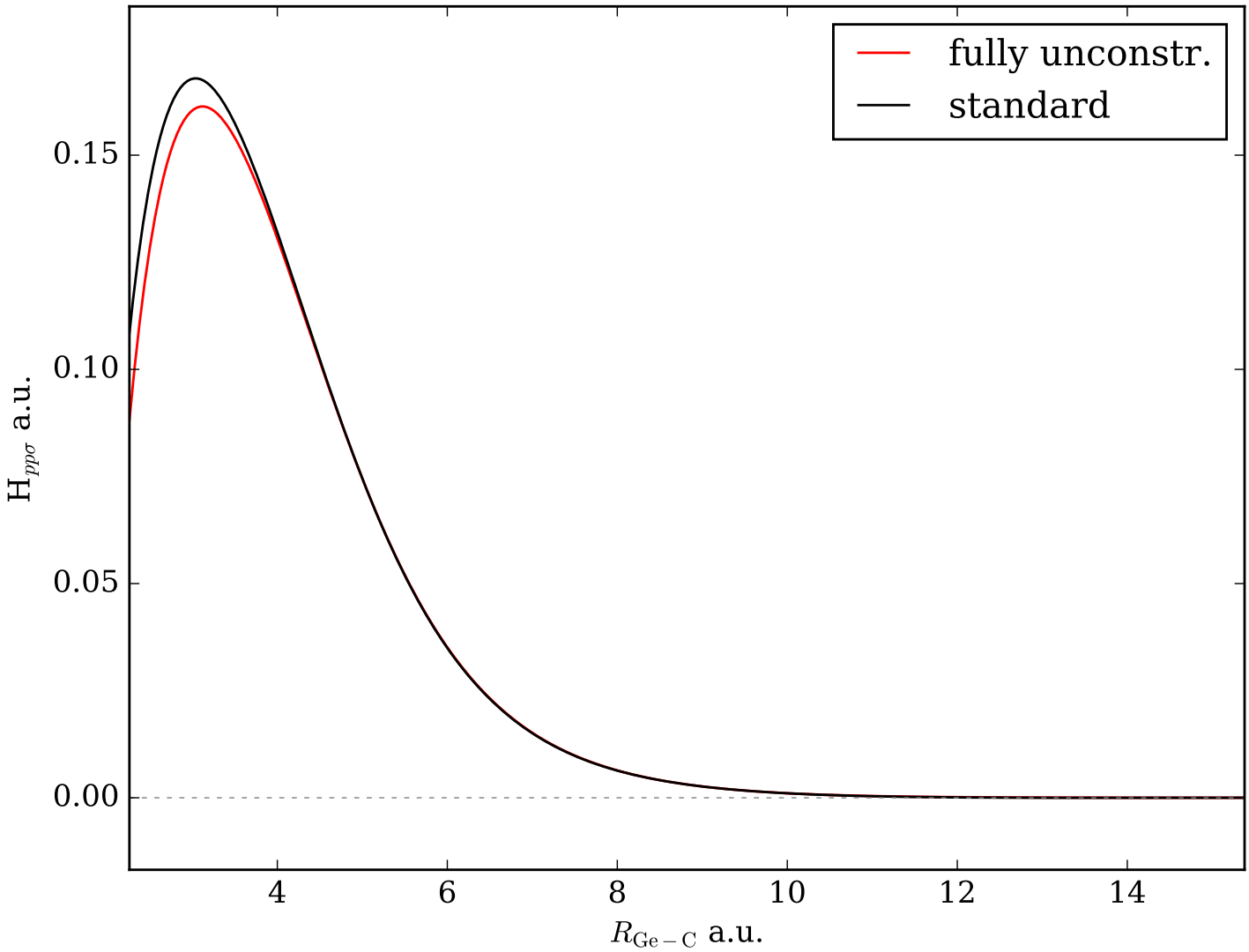

fully unconstr.
standard
0.4
0.3
0.2
0.1
0.0
$S_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Ge}}$ a.u.

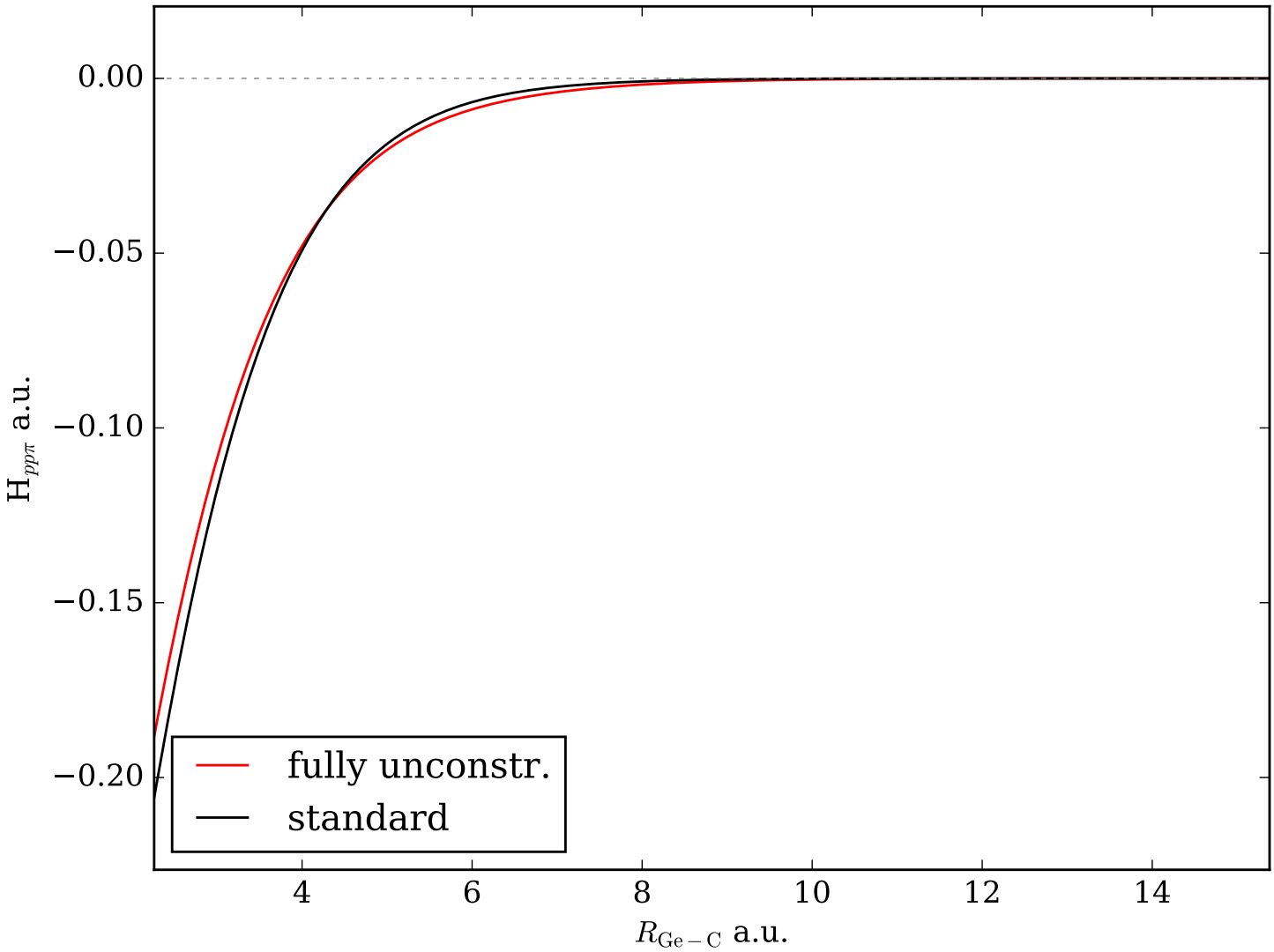
7.2 Repulsive

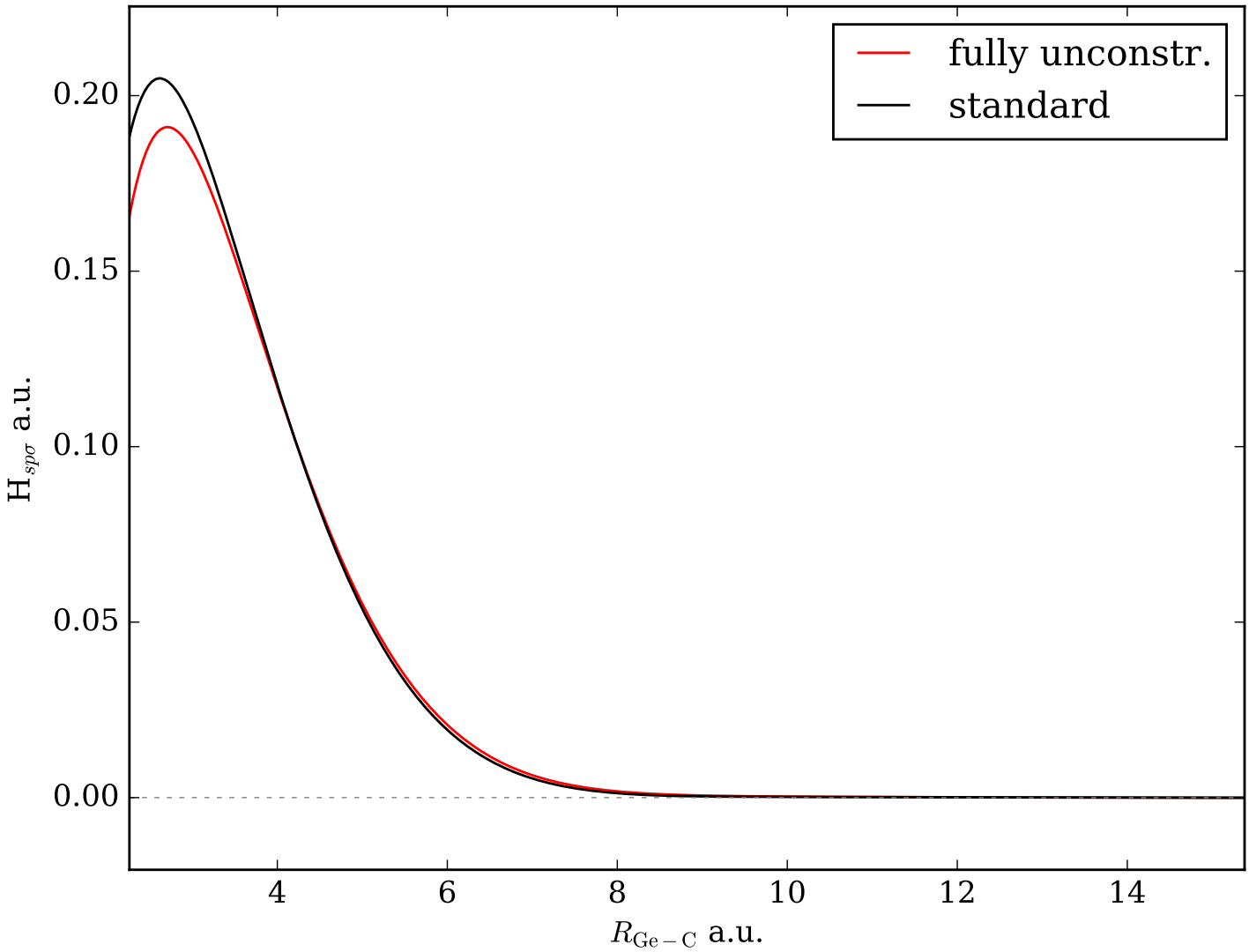


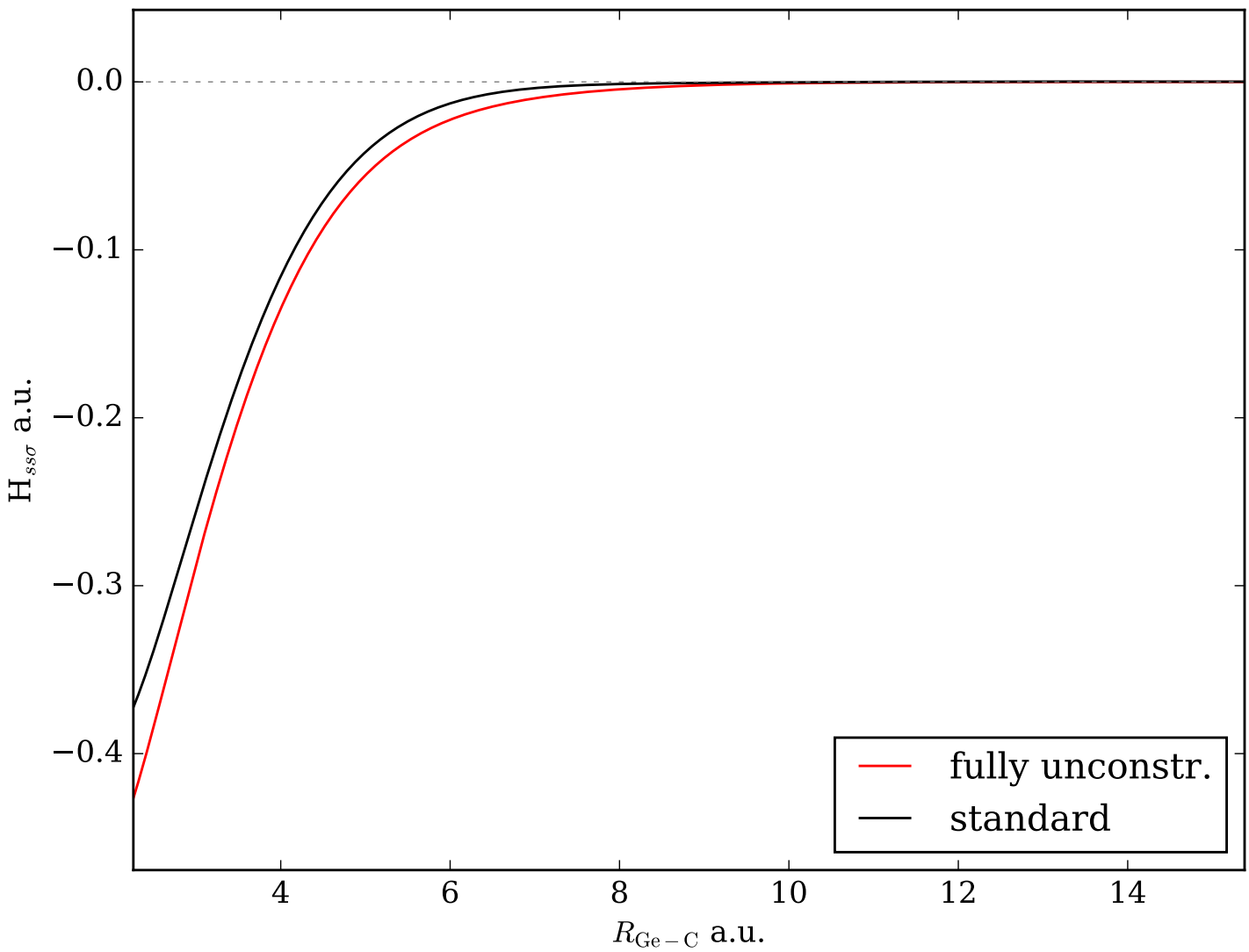
8 Ge-C

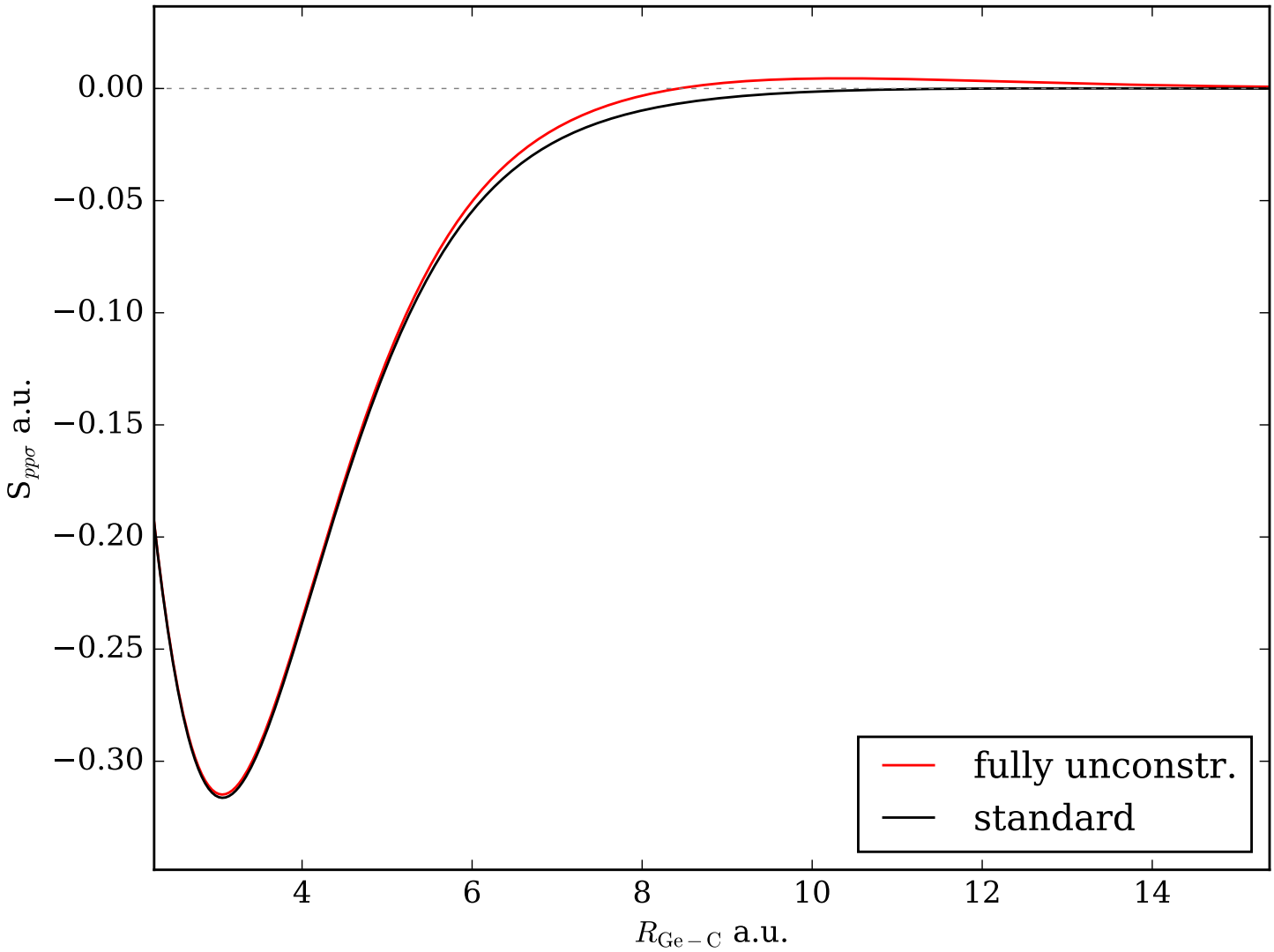
8.1 Electronic

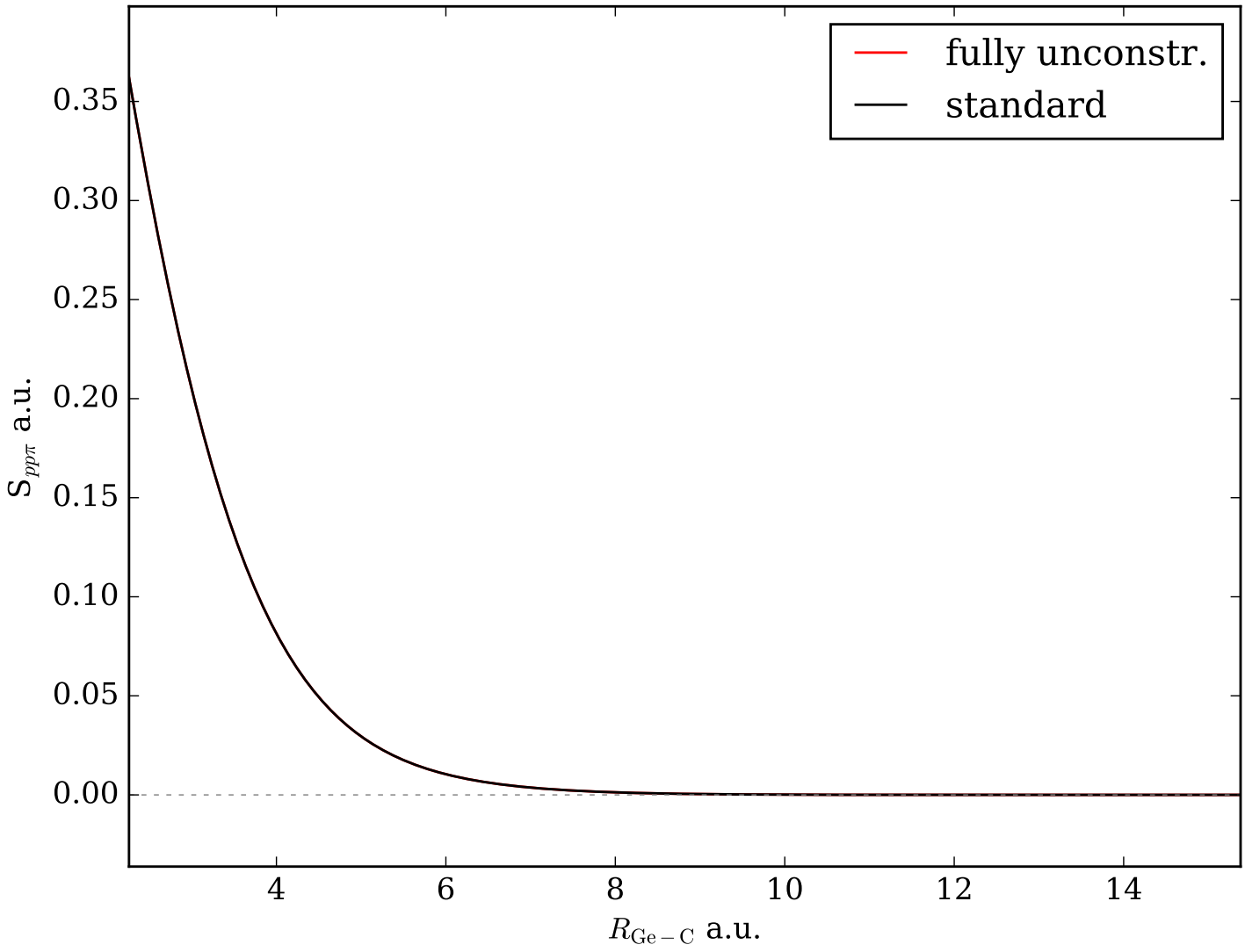


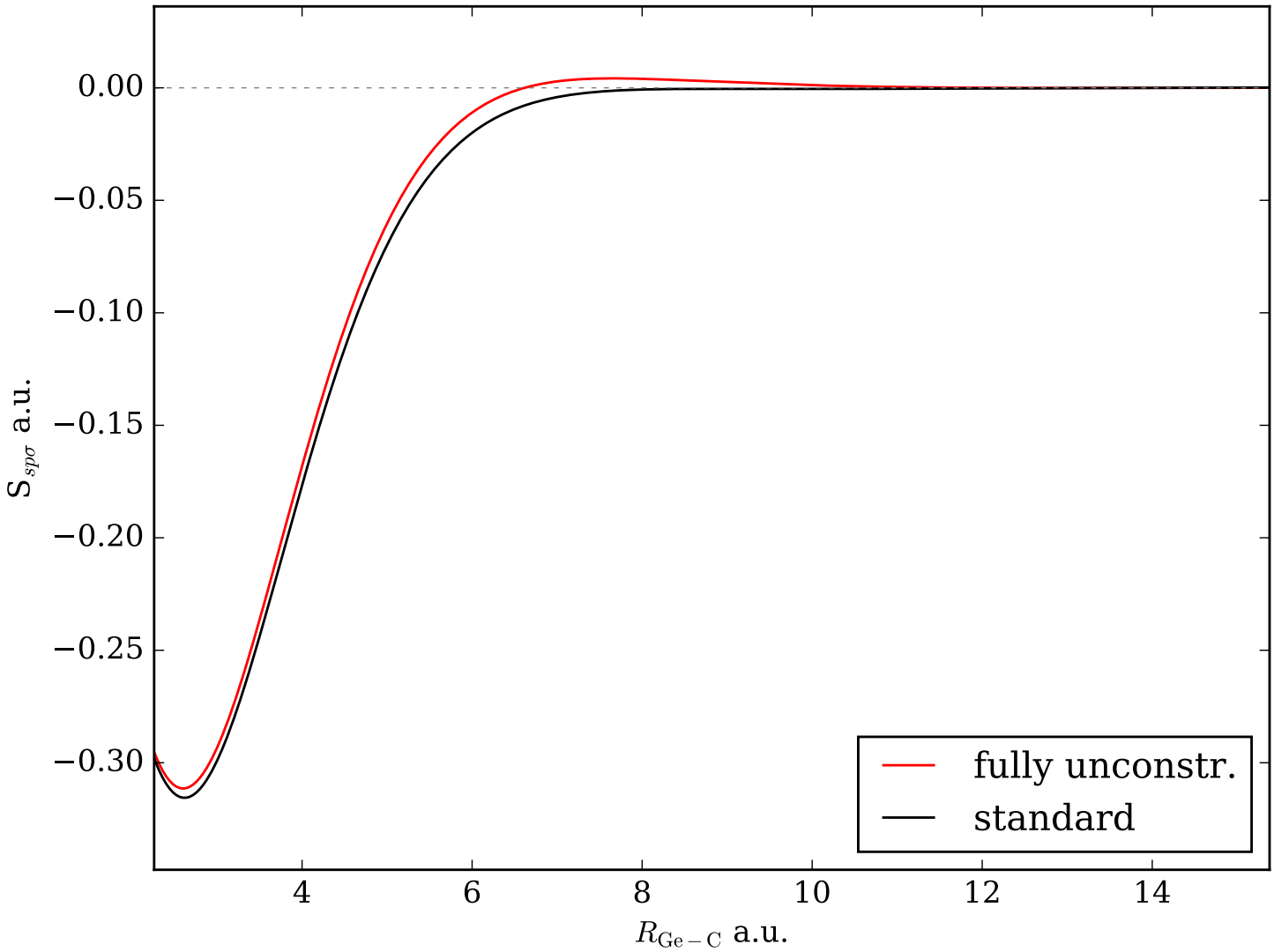

0.00
−0.05
−0.10
−0.15
−0.20
$H_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-C}}$ a.u.
fully unconstr.
standard

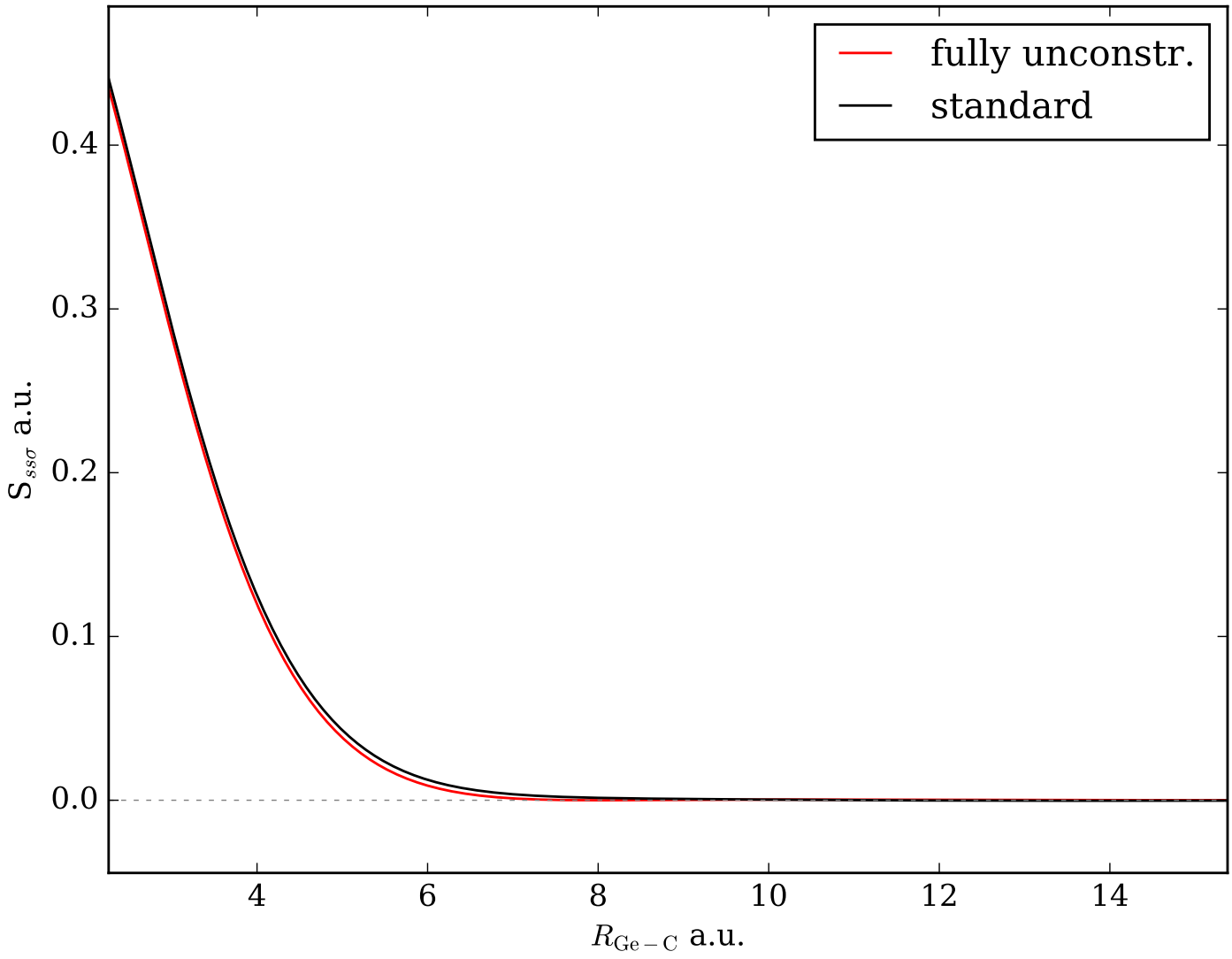

fully unconstr.
standard
0.20
0.15
0.10
0.05
0.00
$H_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-C}}$ a.u.


0.0
−0.1
−0.2
−0.3
−0.4
$H_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-C}}$ a.u.
fully unconstr.
standard


0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
$S_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-C}}$ a.u.
fully unconstr.
standard

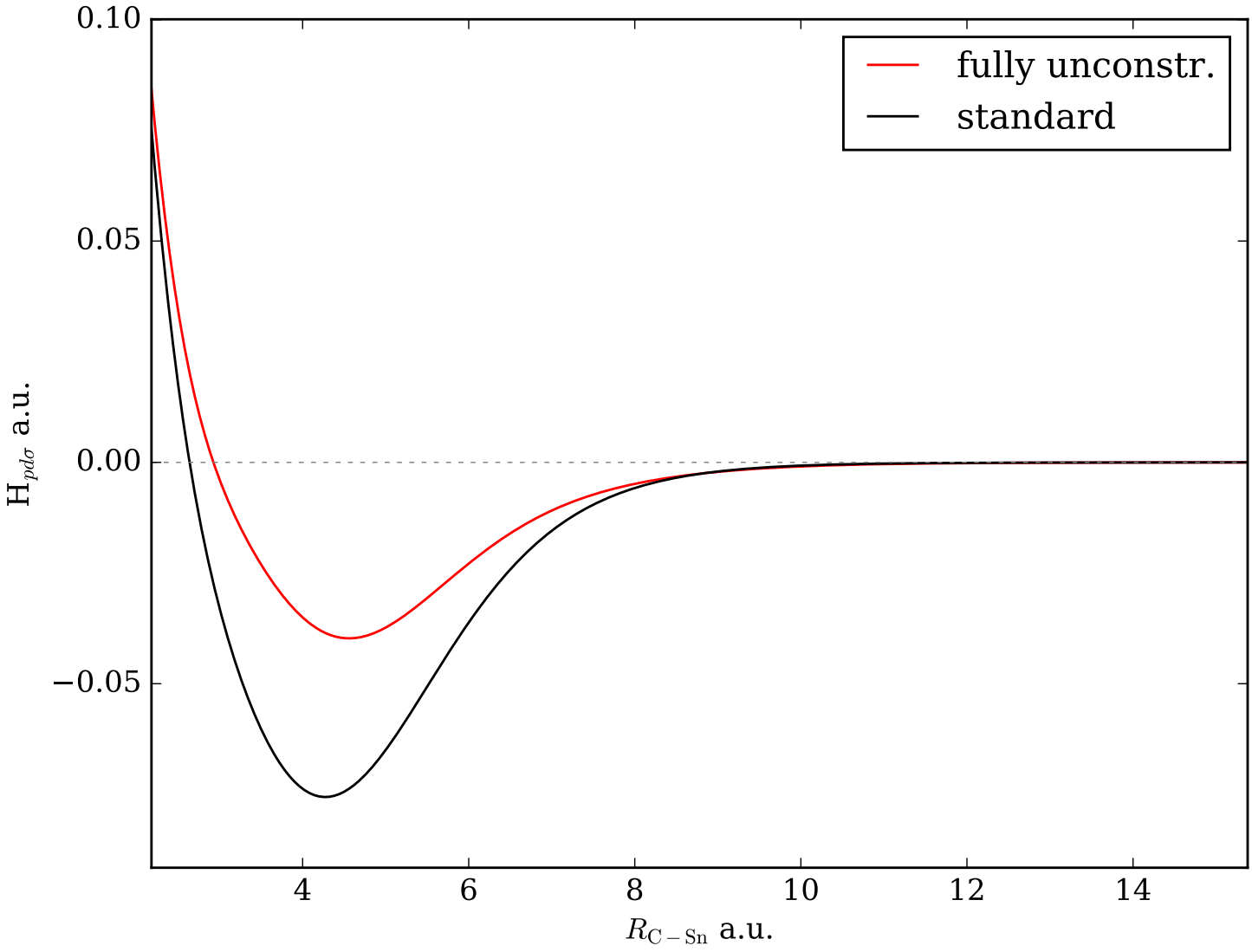

fully unconstr.
standard
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$S_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-C}}$ a.u.

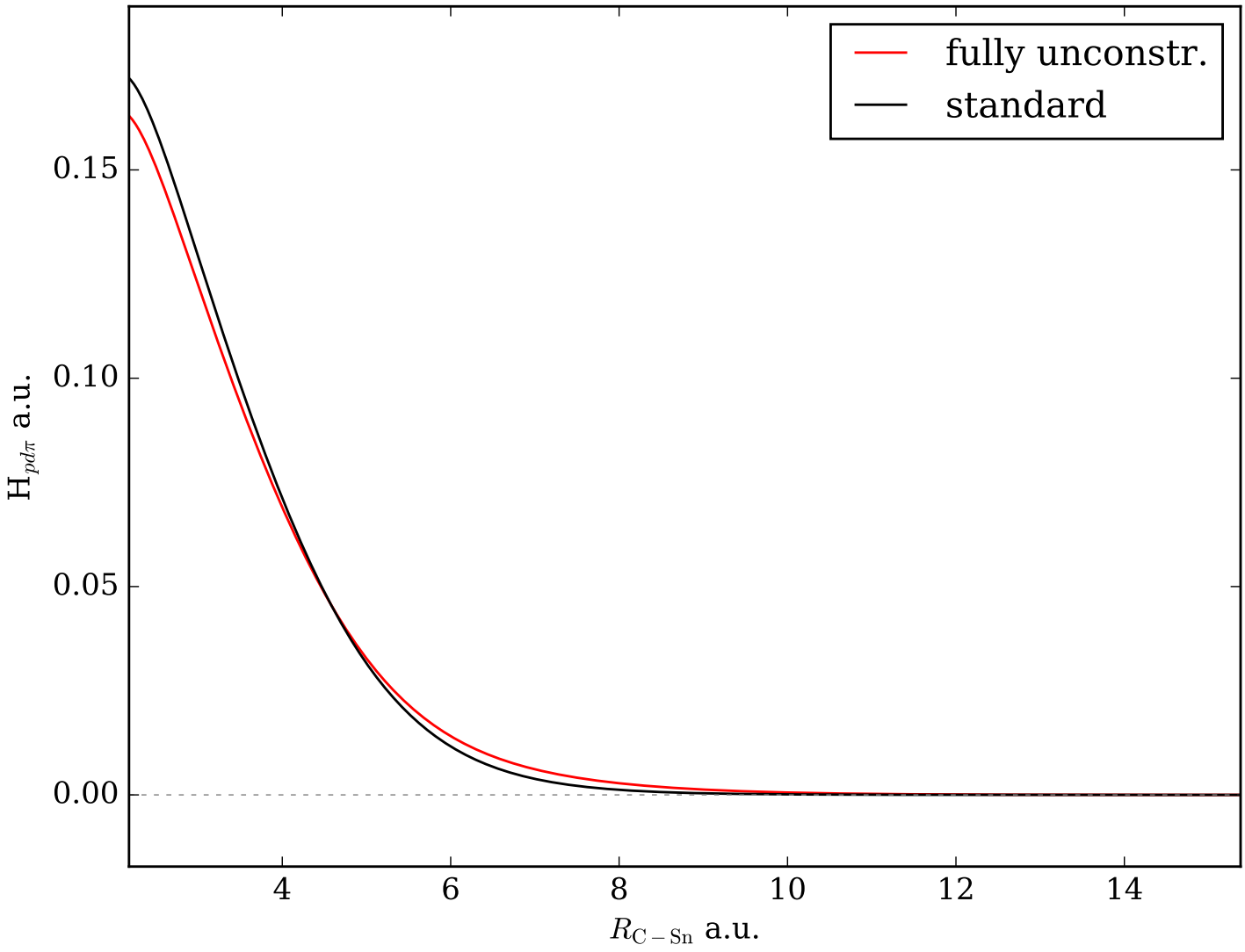

0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
$S_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-C}}$ a.u.
fully unconstr.
standard

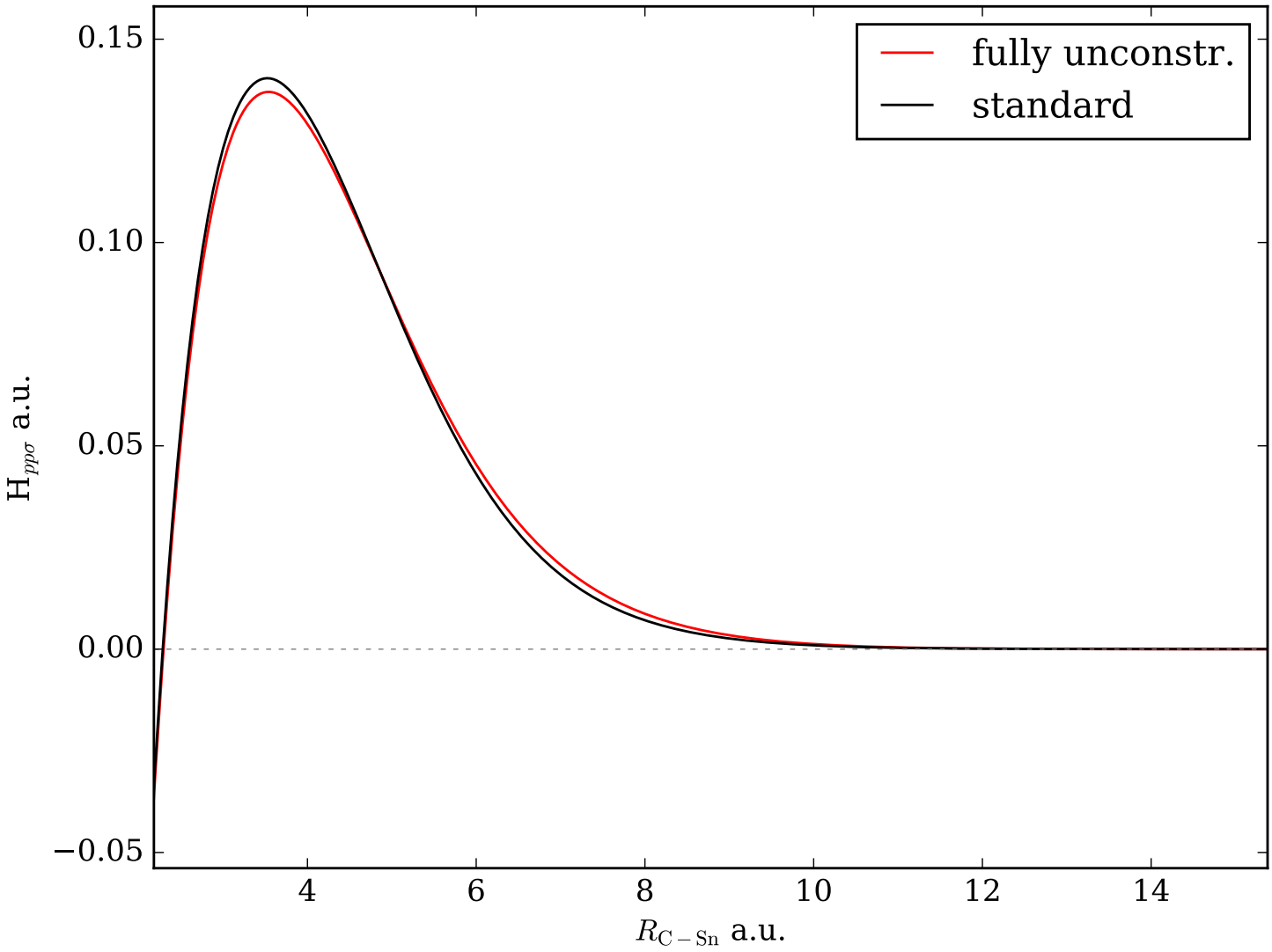

fully unconstr.
standard
0.4
0.3
0.2
0.1
0.0
$S_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-C}}$ a.u.

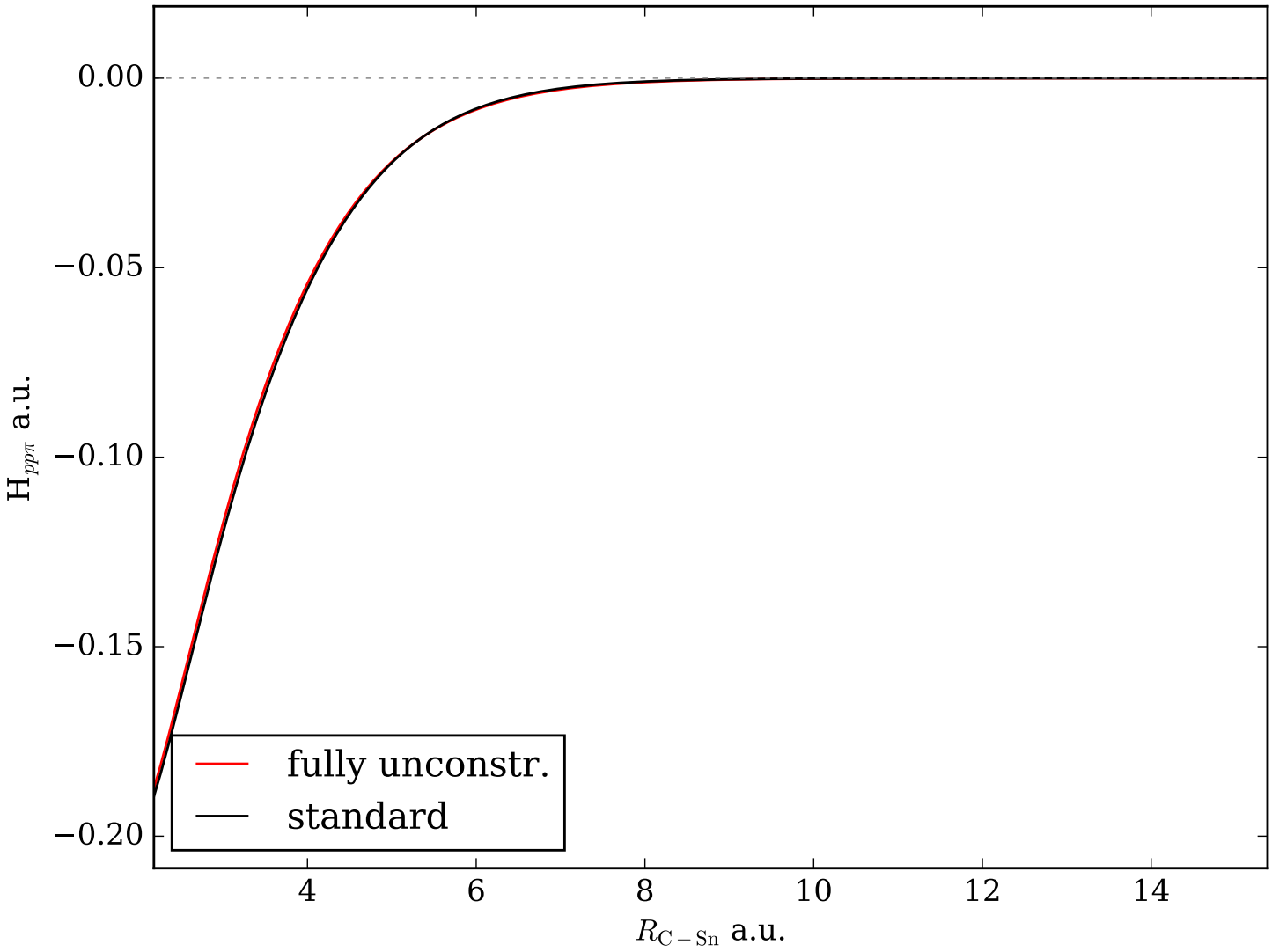
9 C-Sn

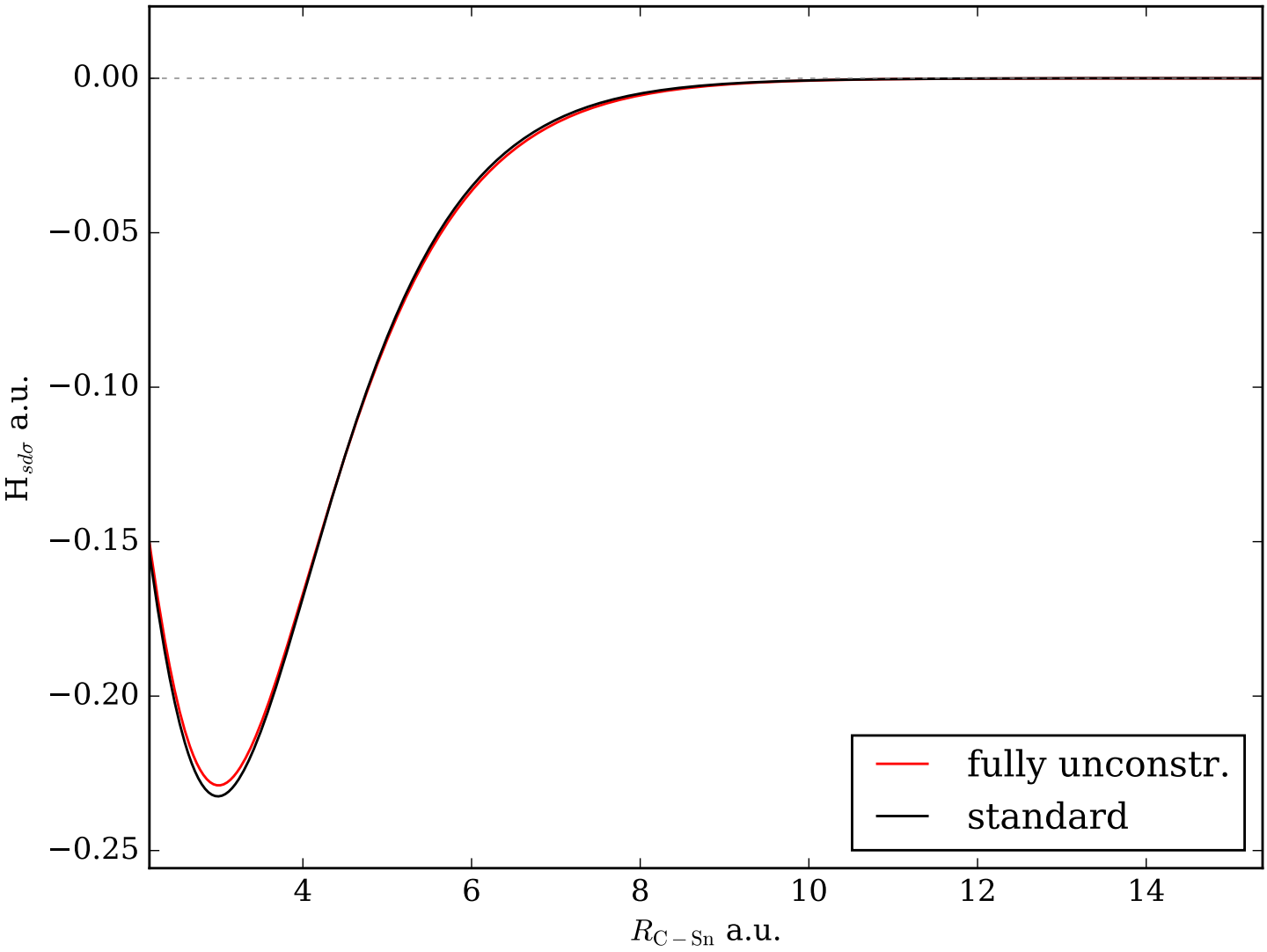
9.1 Electronic

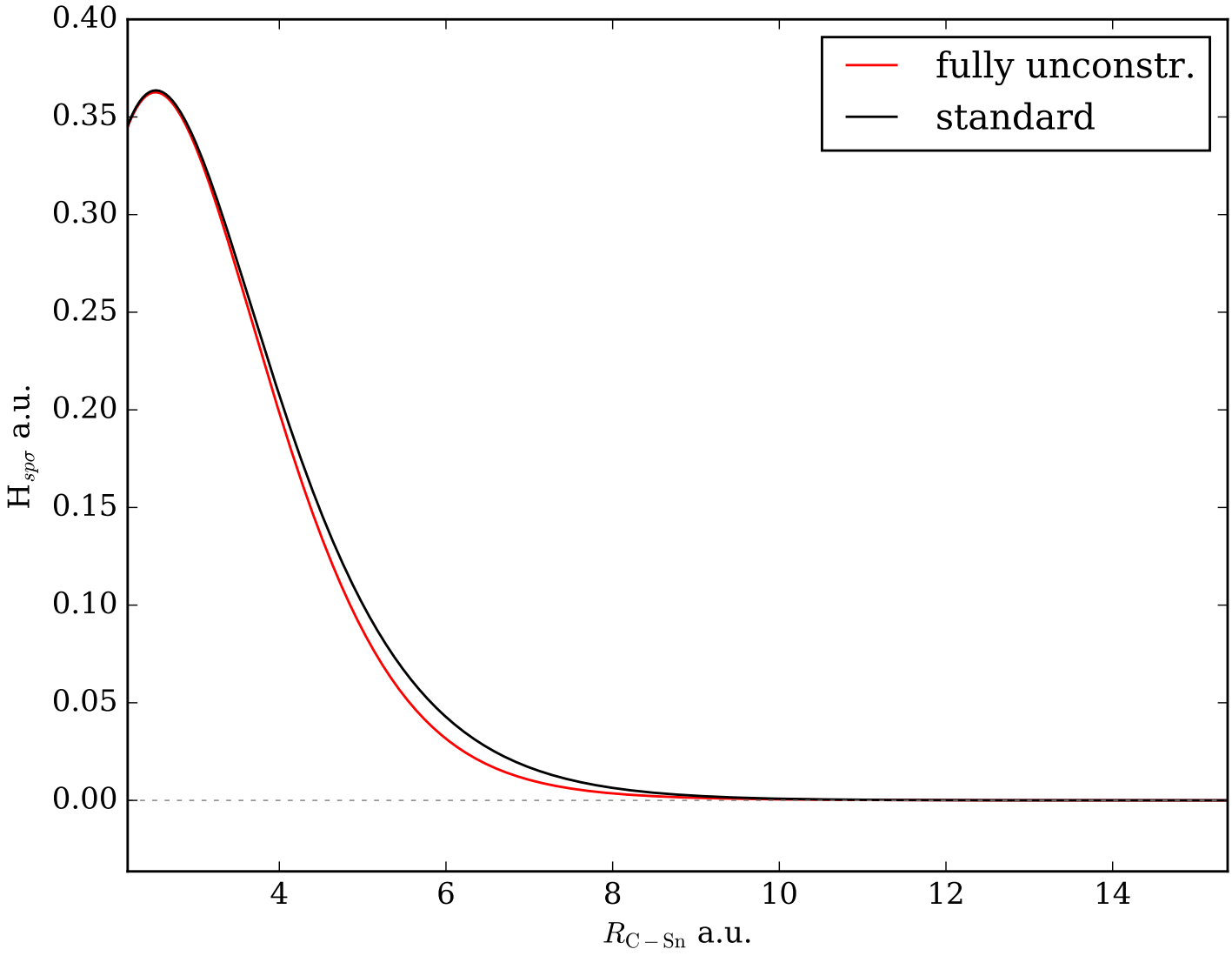


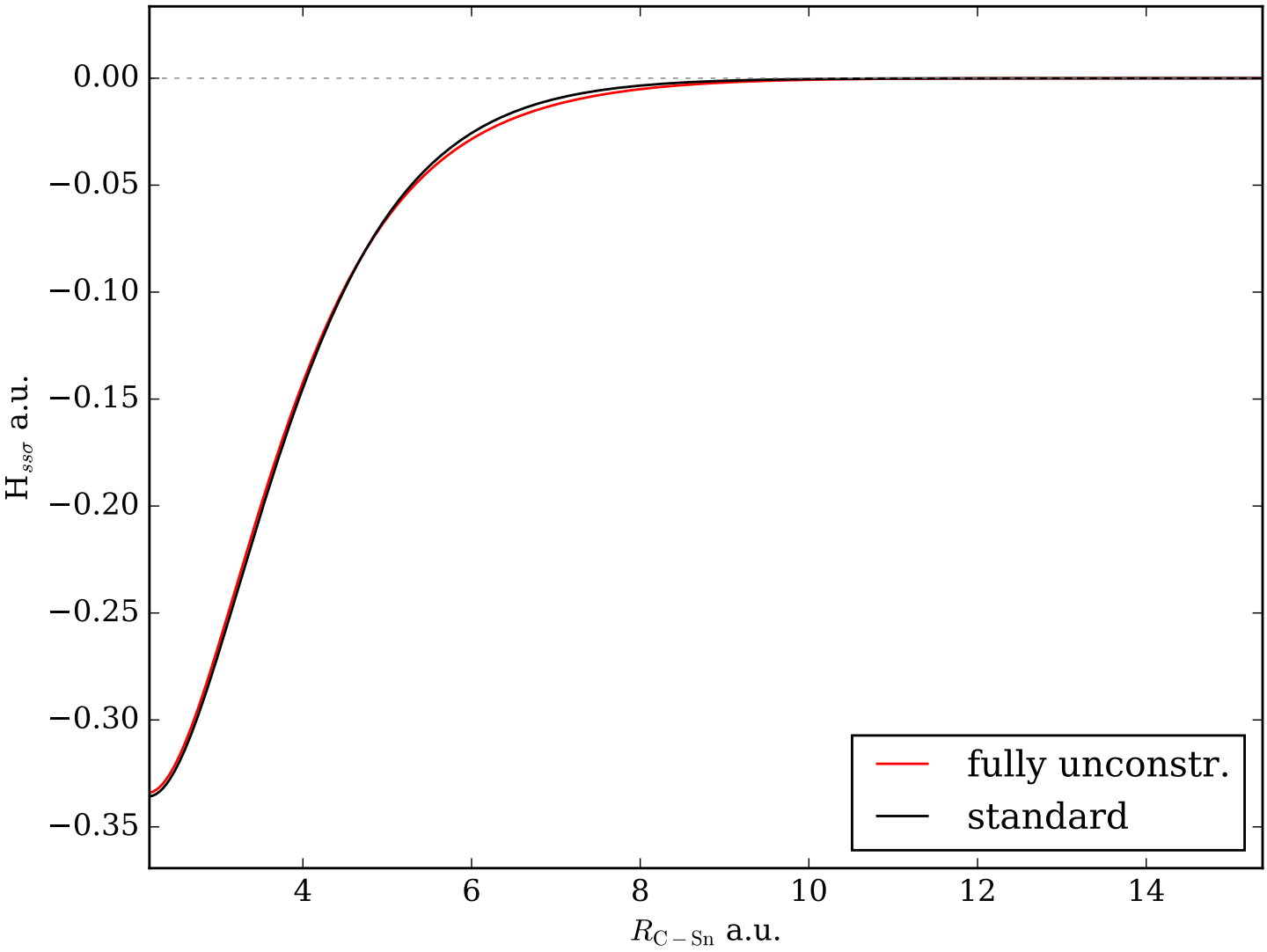

fully unconstr.
standard
0.15
0.10
0.05
0.00
$H_{pd\pi}$ a.u.
4
6
8
10
12
14
R_{C-Sn} a.u.

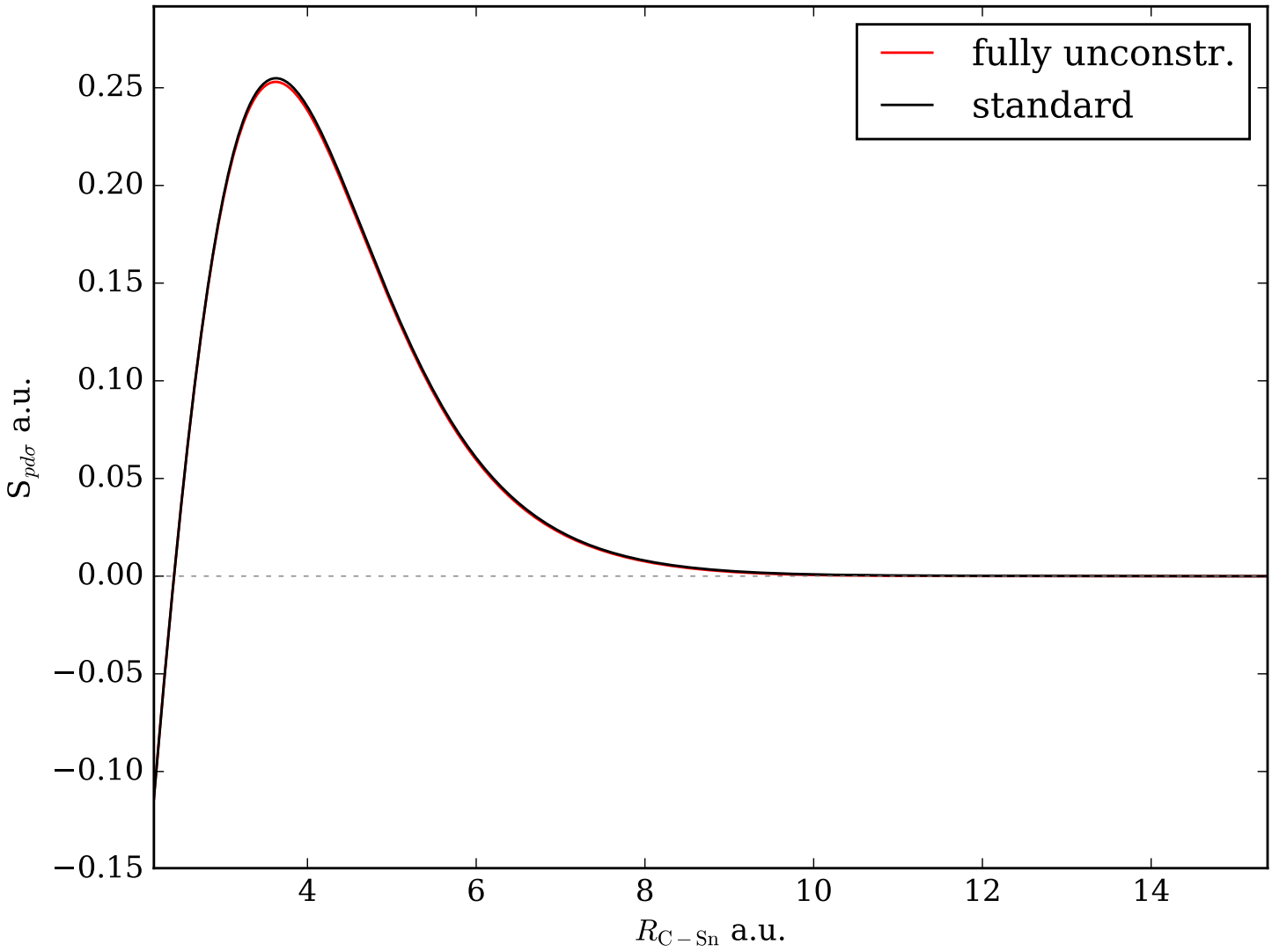

fully unconstr.
standard
0.15
0.10
0.05
0.00
−0.05
4
6
8
10
12
14
$H_{pp\sigma}$ a.u.
R_{C-Sn} a.u.

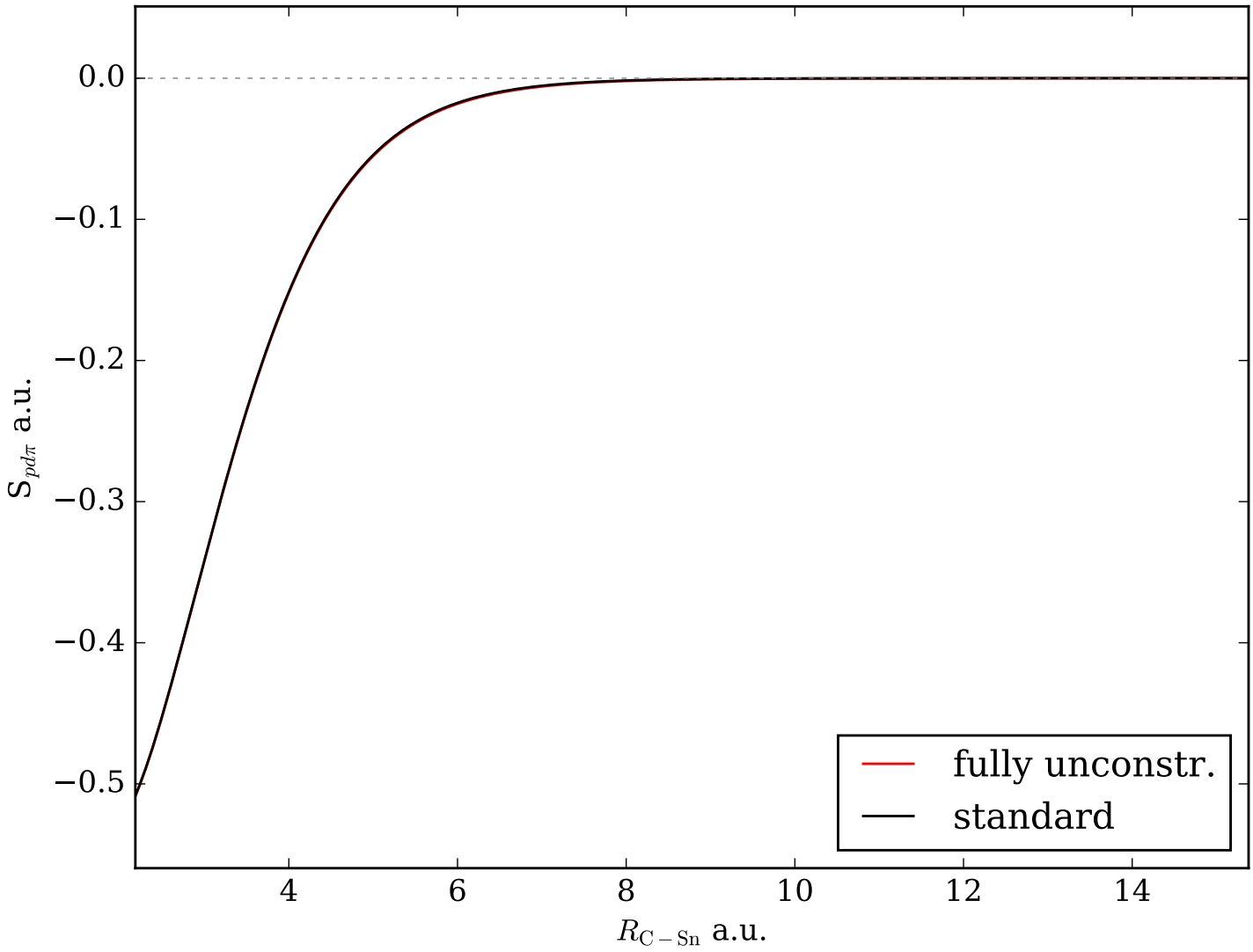

0.00
−0.05
−0.10
−0.15
−0.20
$H_{pp\pi}$ a.u.
4
6
8
10
12
14
R_{C-Sn} a.u.
fully unconstr.
standard

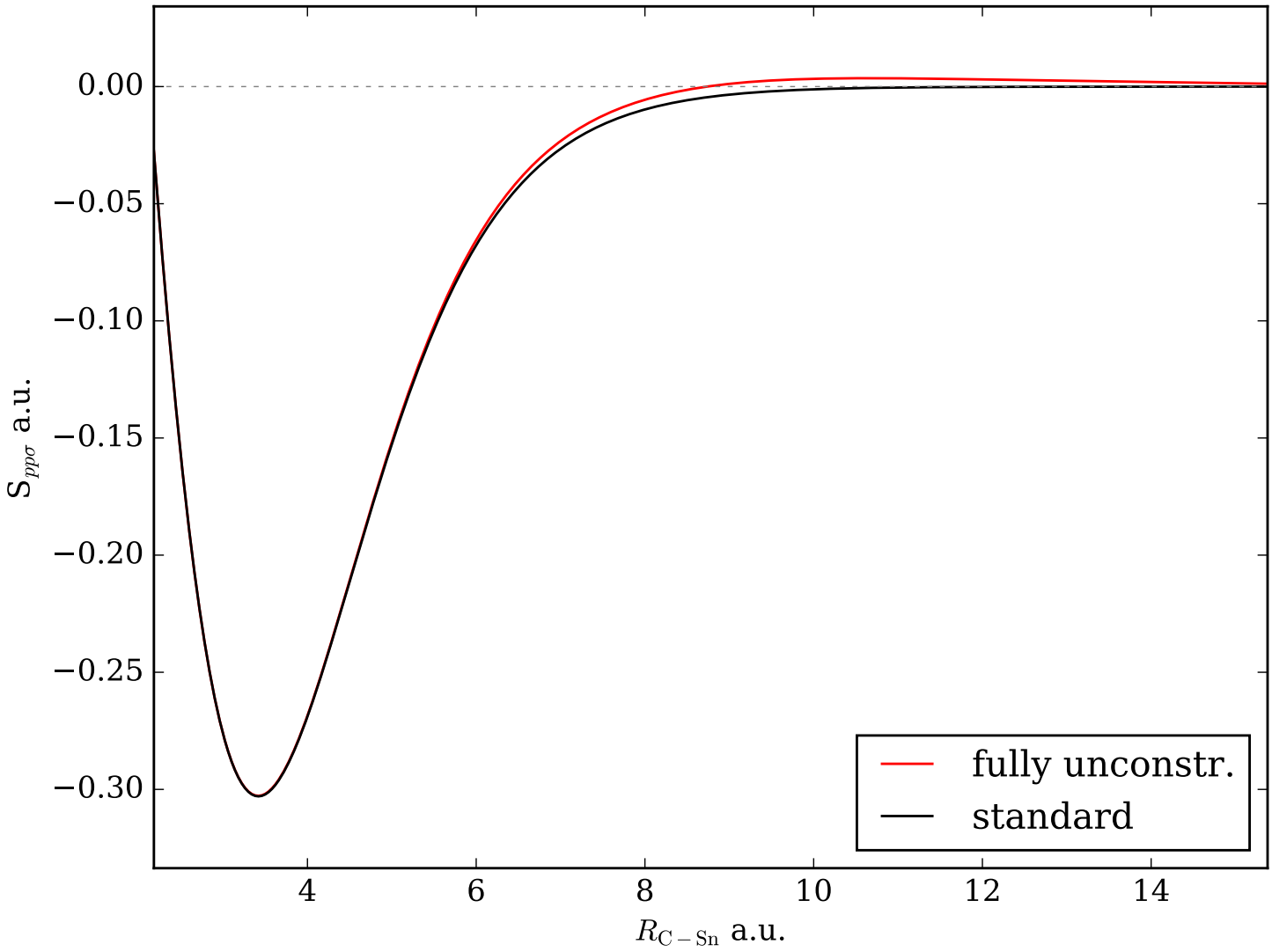

0.00
−0.05
−0.10
−0.15
−0.20
−0.25
$H_{sd\sigma}$ a.u.
4
6
8
10
12
14
R_{C-Sn} a.u.
fully unconstr.
standard

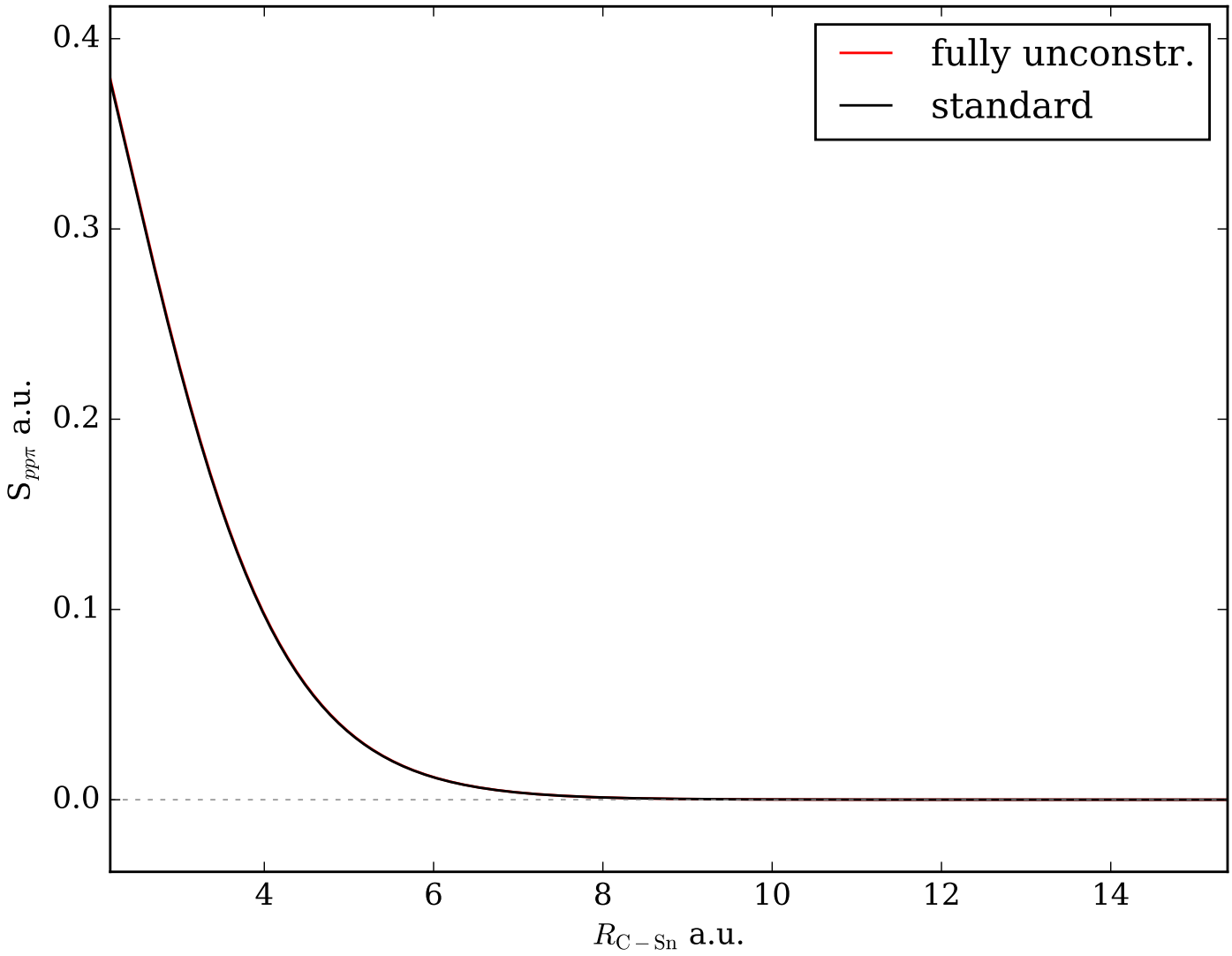

fully unconstr.
standard
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$H_{sp\sigma}$ a.u.
4
6
8
10
12
14
R_{C-Sn} a.u.

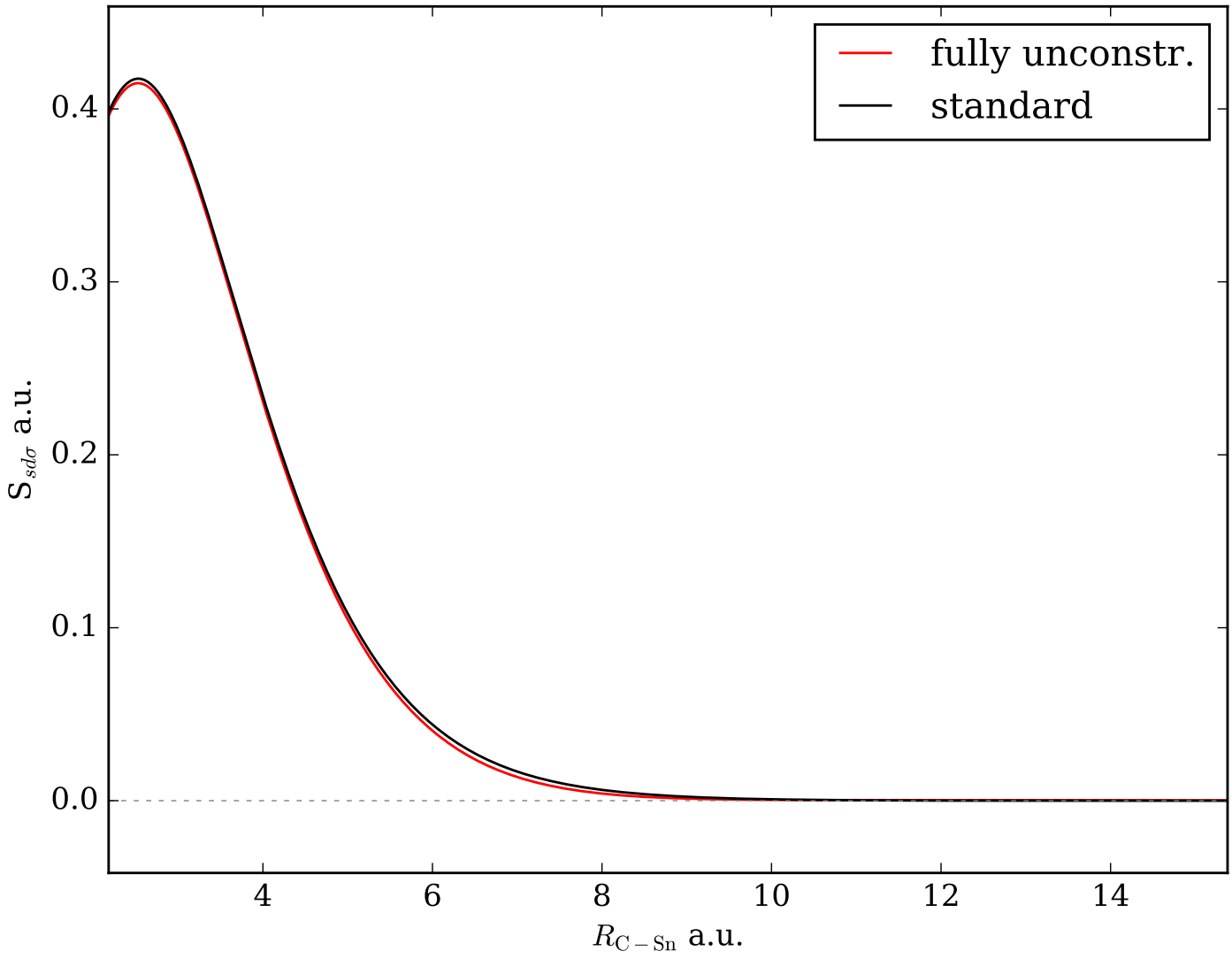

0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
−0.35
$H_{ss\sigma}$ a.u.
4
6
8
10
12
14
R_{C-Sn} a.u.
fully unconstr.
standard

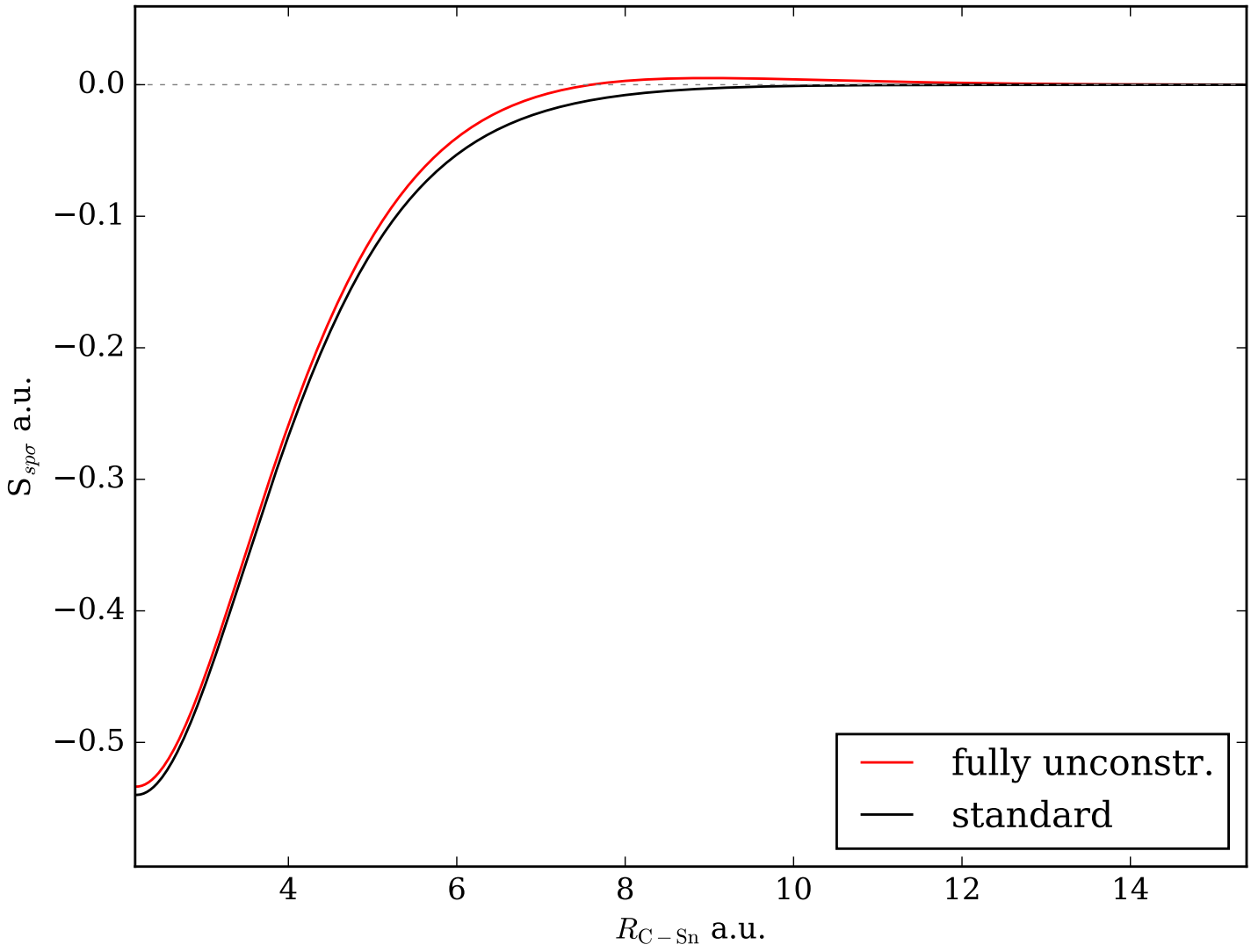

fully unconstr.
standard
0.25
0.20
0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
$S_{pd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Sn}}$ a.u.

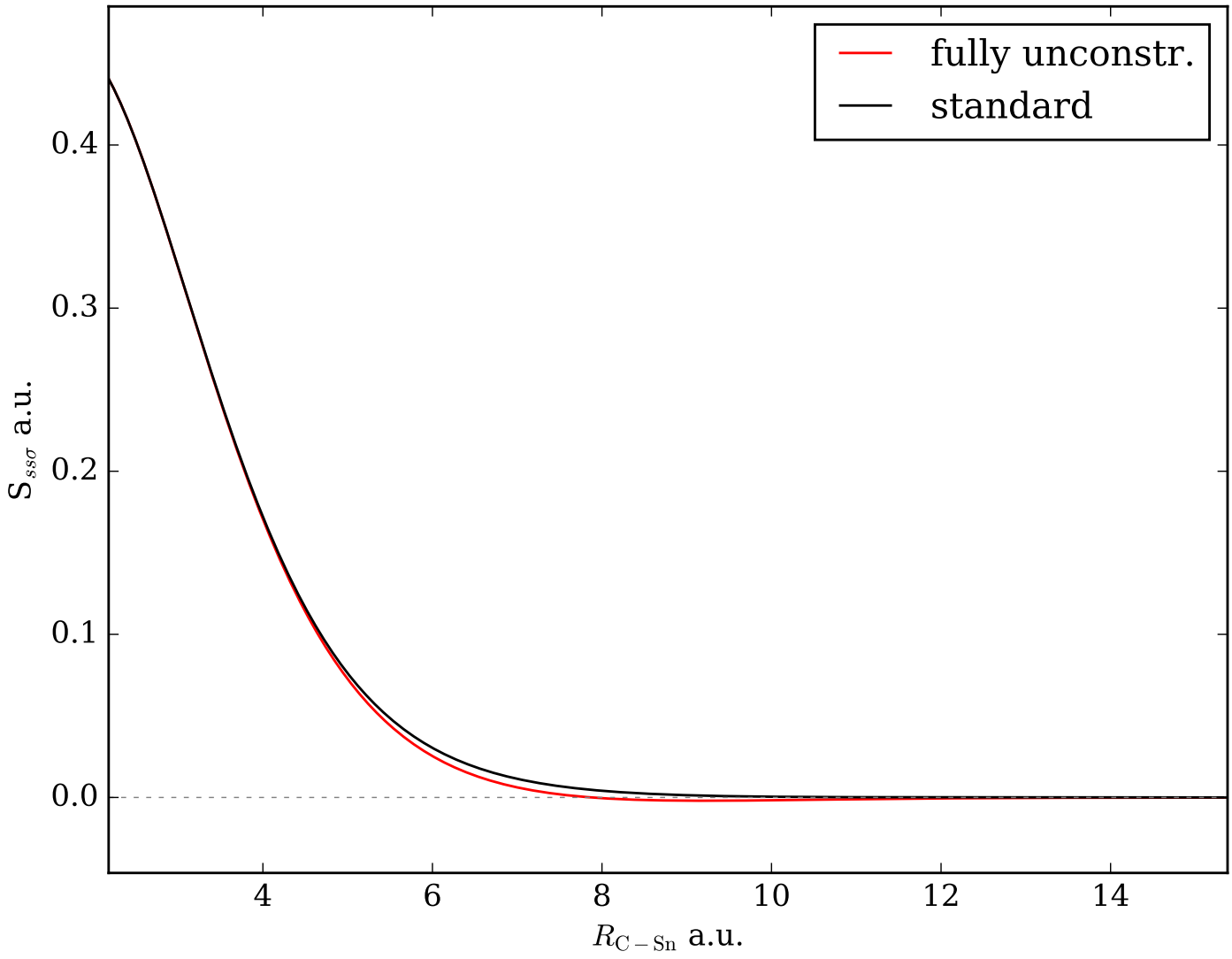

0.0
−0.1
−0.2
−0.3
−0.4
−0.5
$S_{pd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Sn}}$ a.u.
fully unconstr.
standard


0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
$S_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Sn}}$ a.u.
fully unconstr.
standard

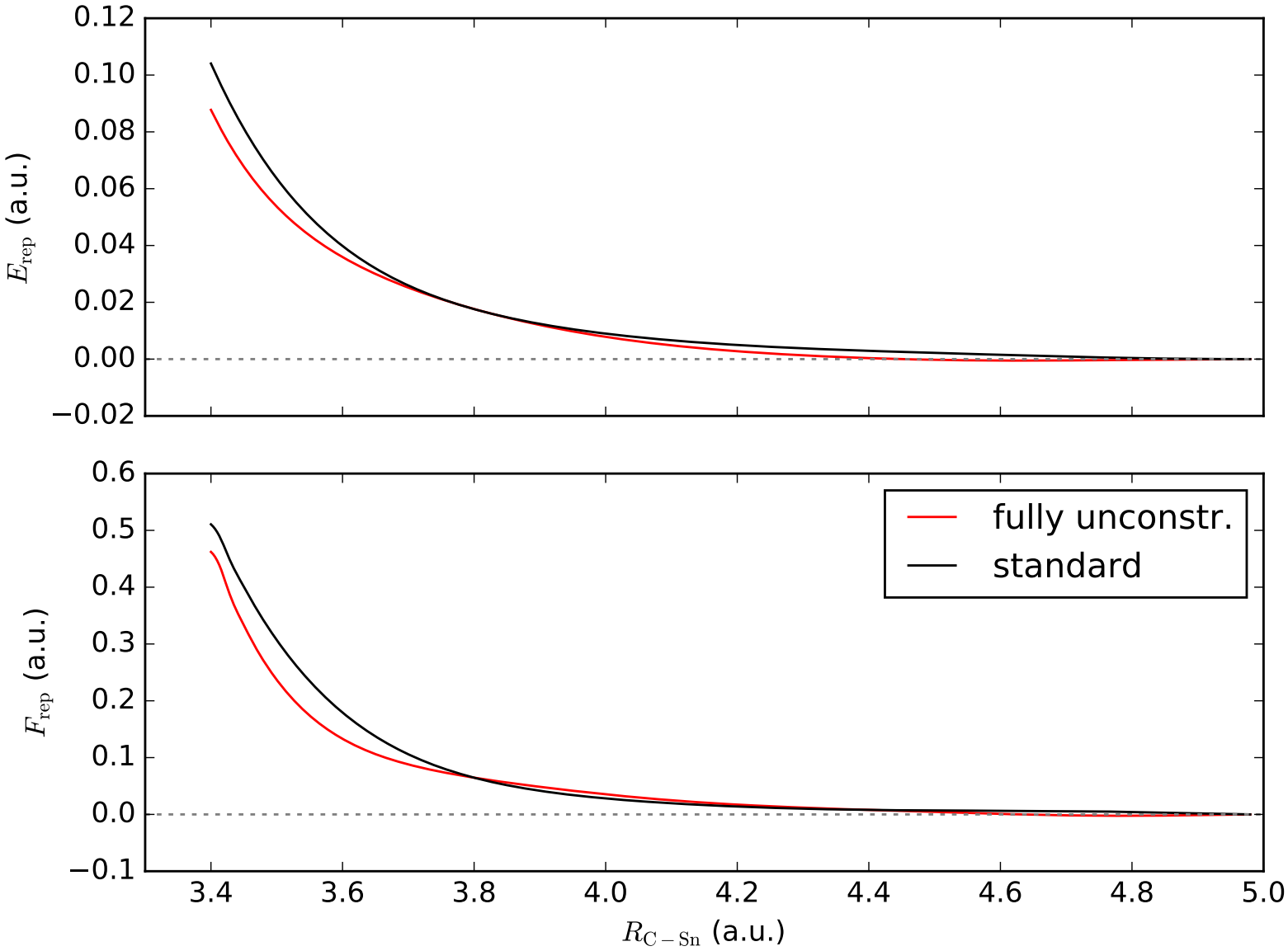

fully unconstr.
standard
0.4
0.3
0.2
0.1
0.0
$S_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Sn}}$ a.u.


fully unconstr.
standard
0.4
0.3
0.2
0.1
0.0
$S_{sd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Sn}}$ a.u.


0.0
−0.1
−0.2
−0.3
−0.4
−0.5
$S_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Sn}}$ a.u.
fully unconstr.
standard

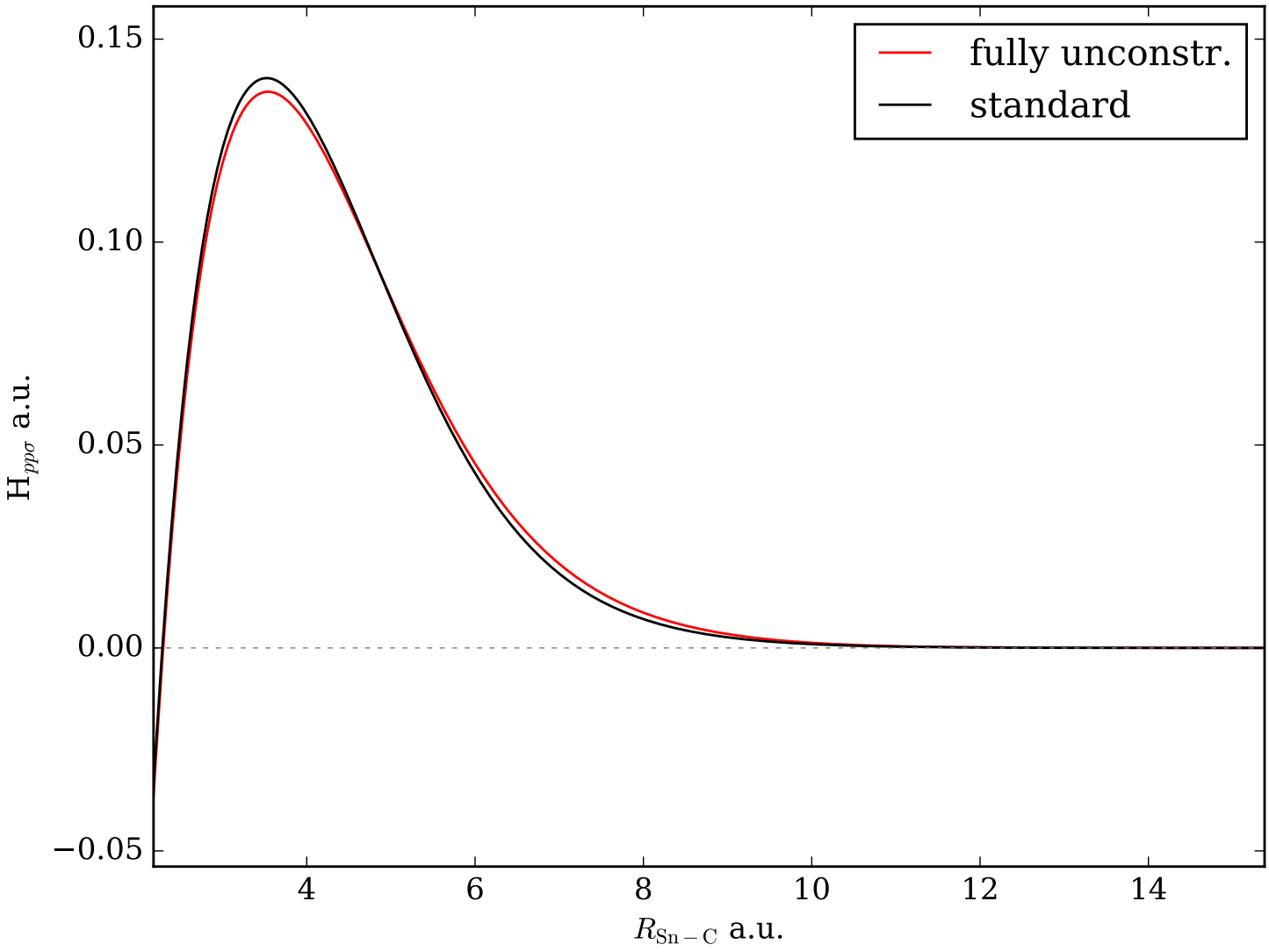

fully unconstr.
standard
0.4
0.3
0.2
0.1
0.0
$S_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{C-Sn}}$ a.u.

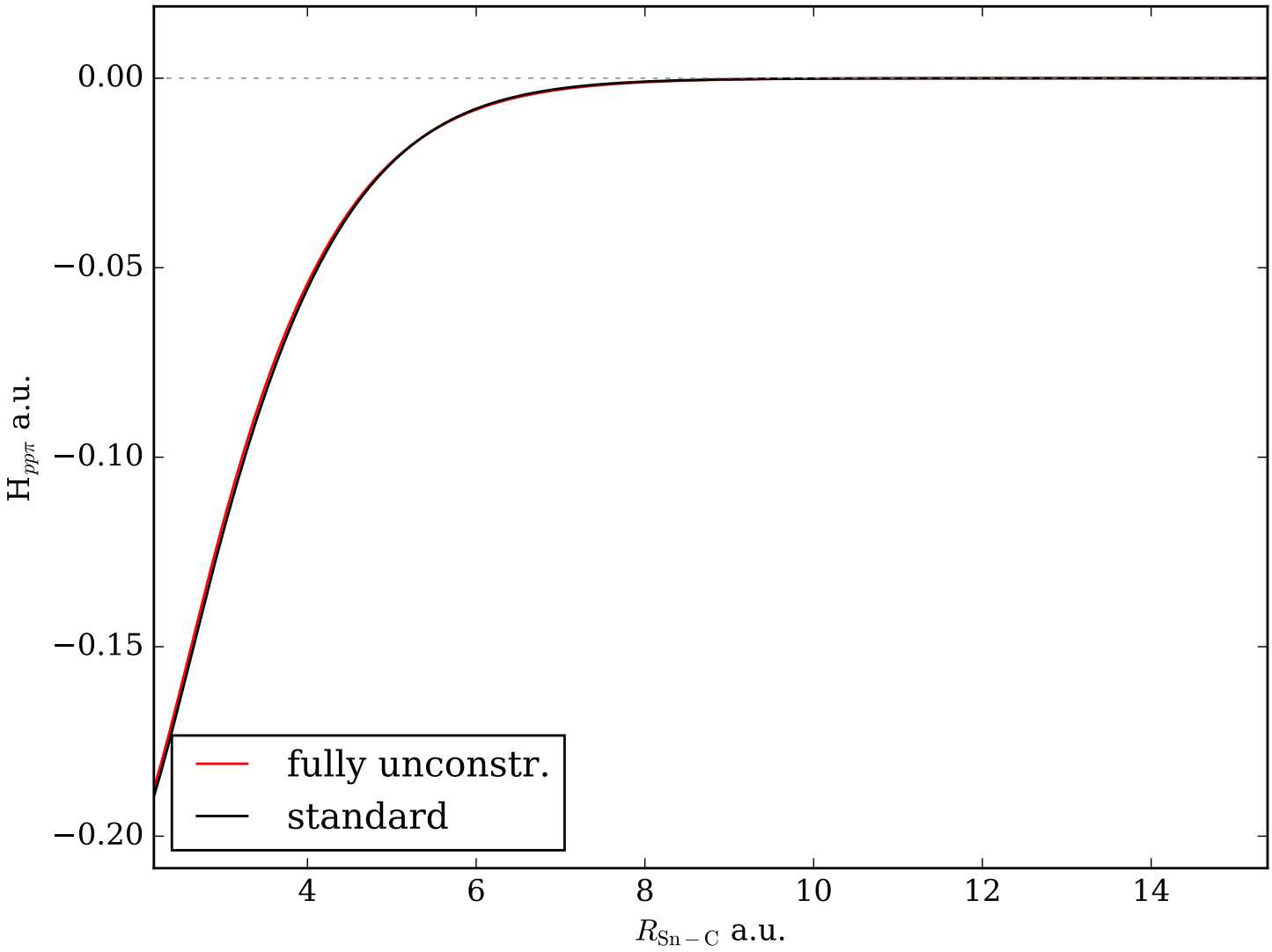
9.2 Repulsive

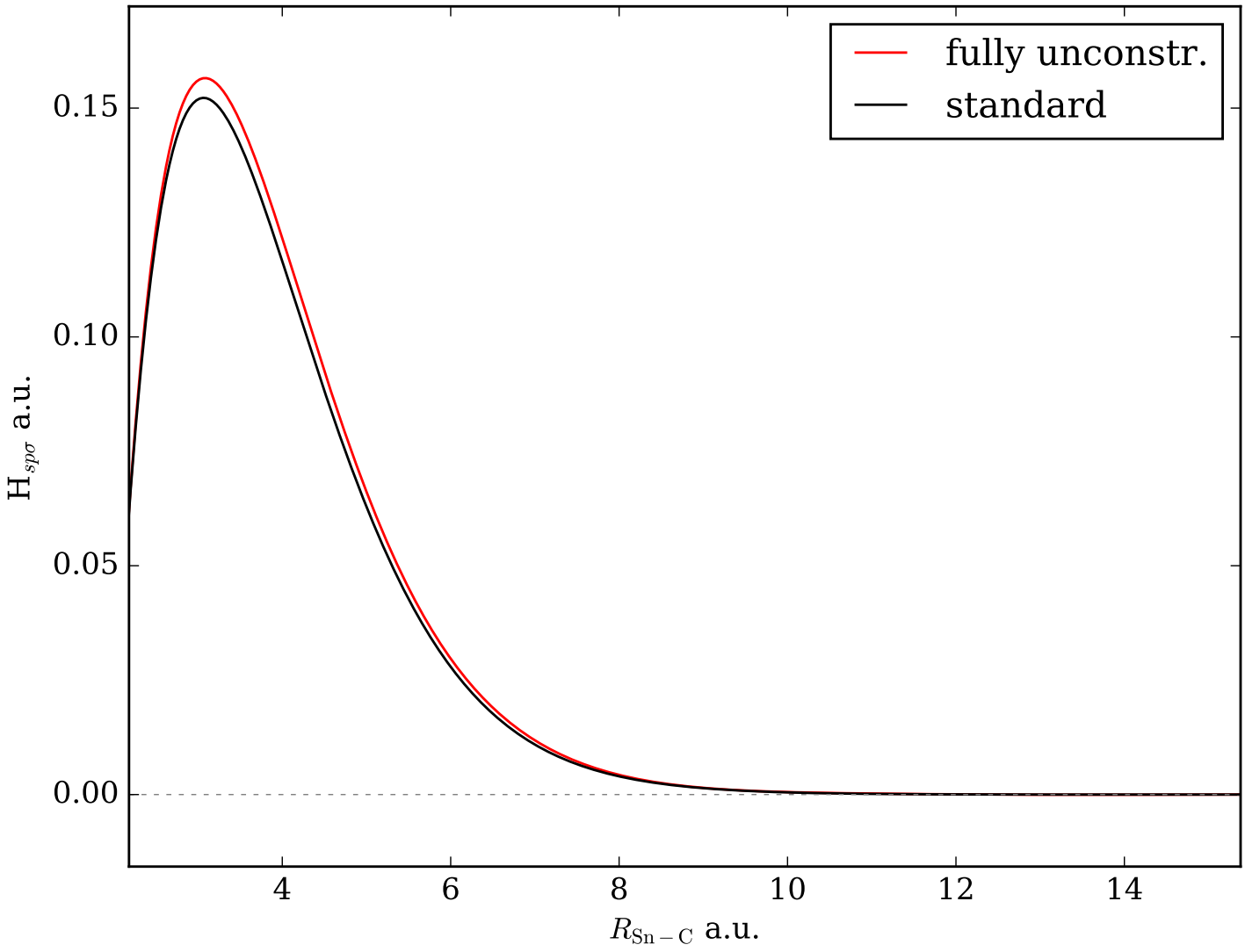


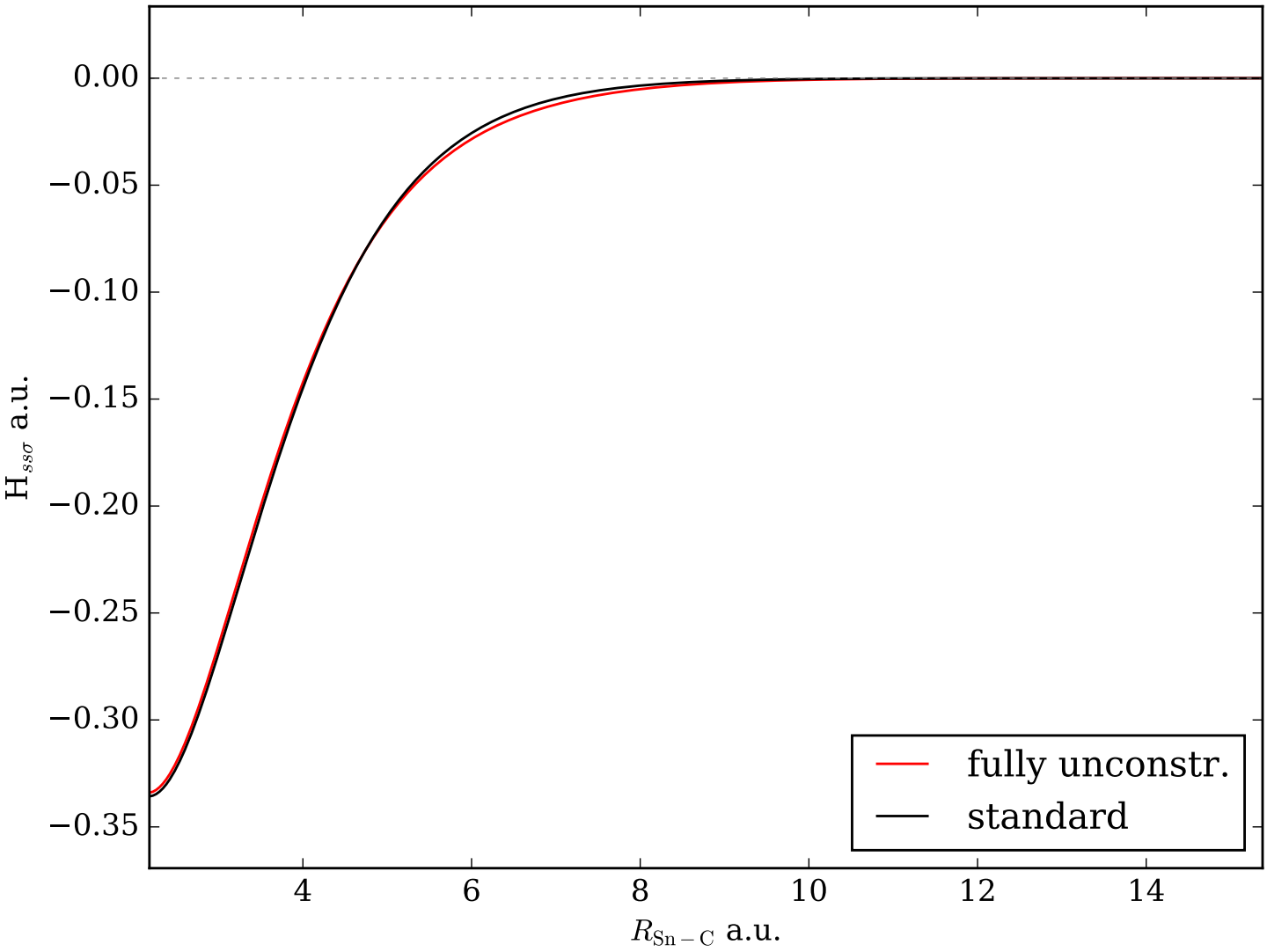
10 Sn-C

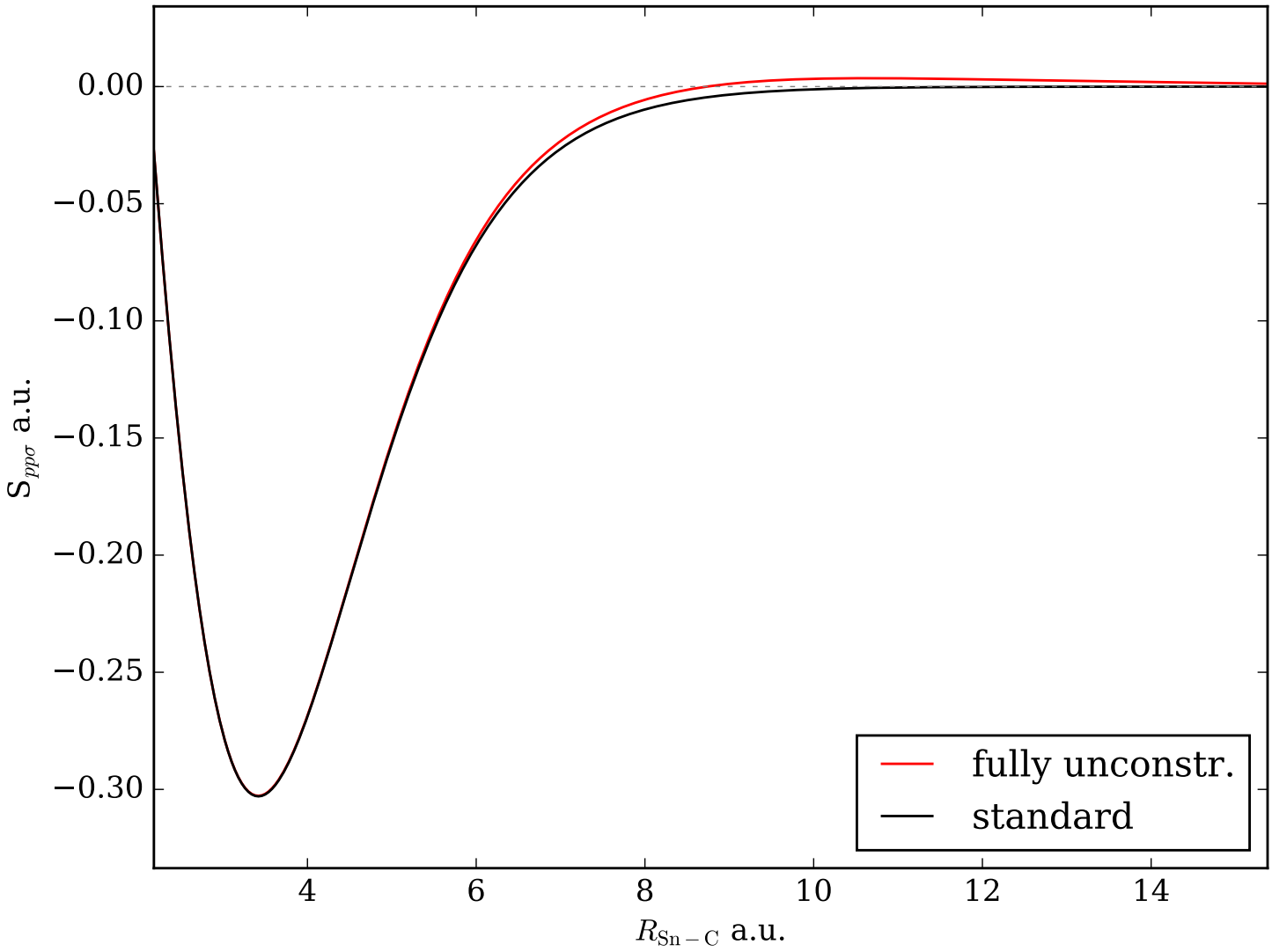
10.1 Electronic

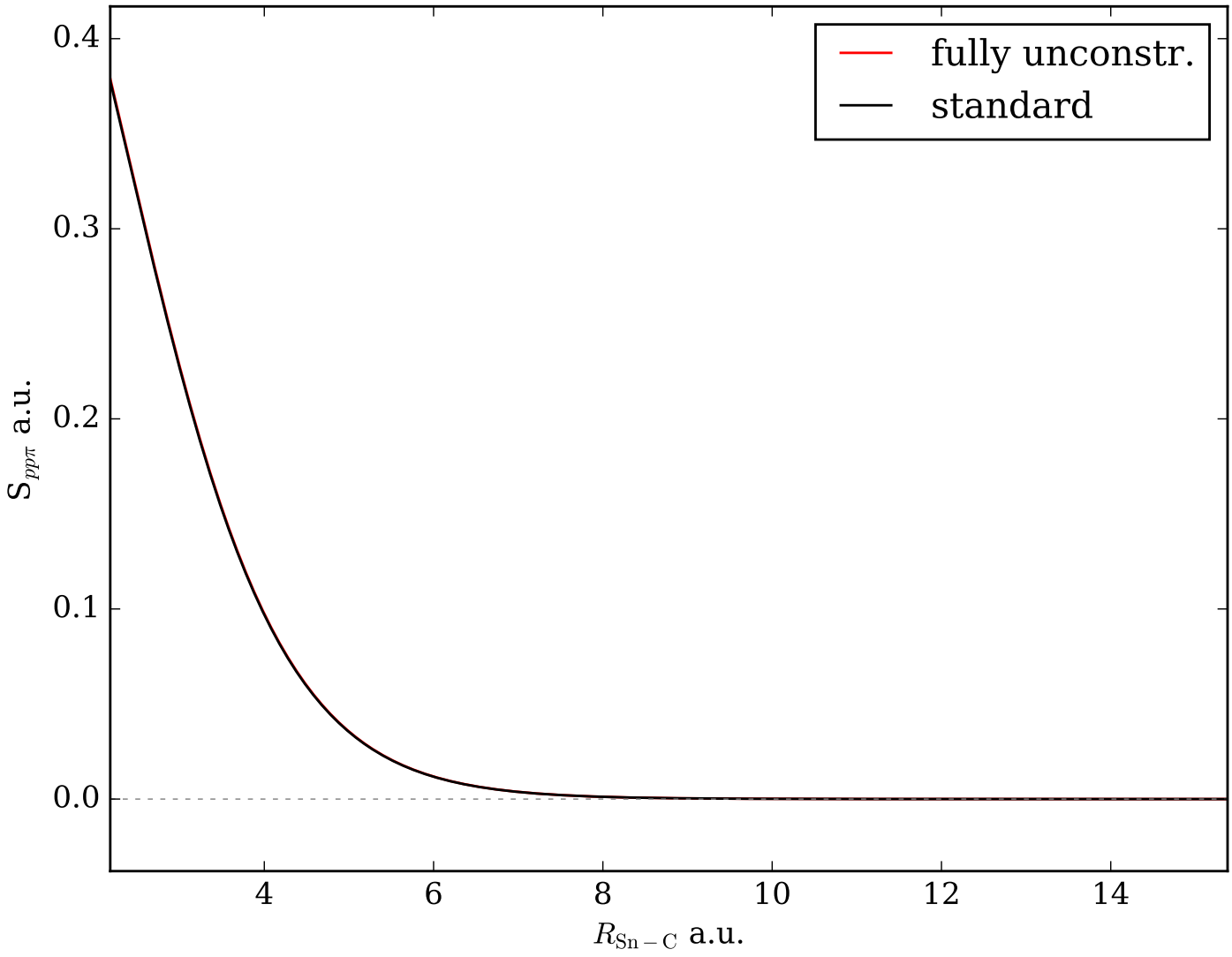


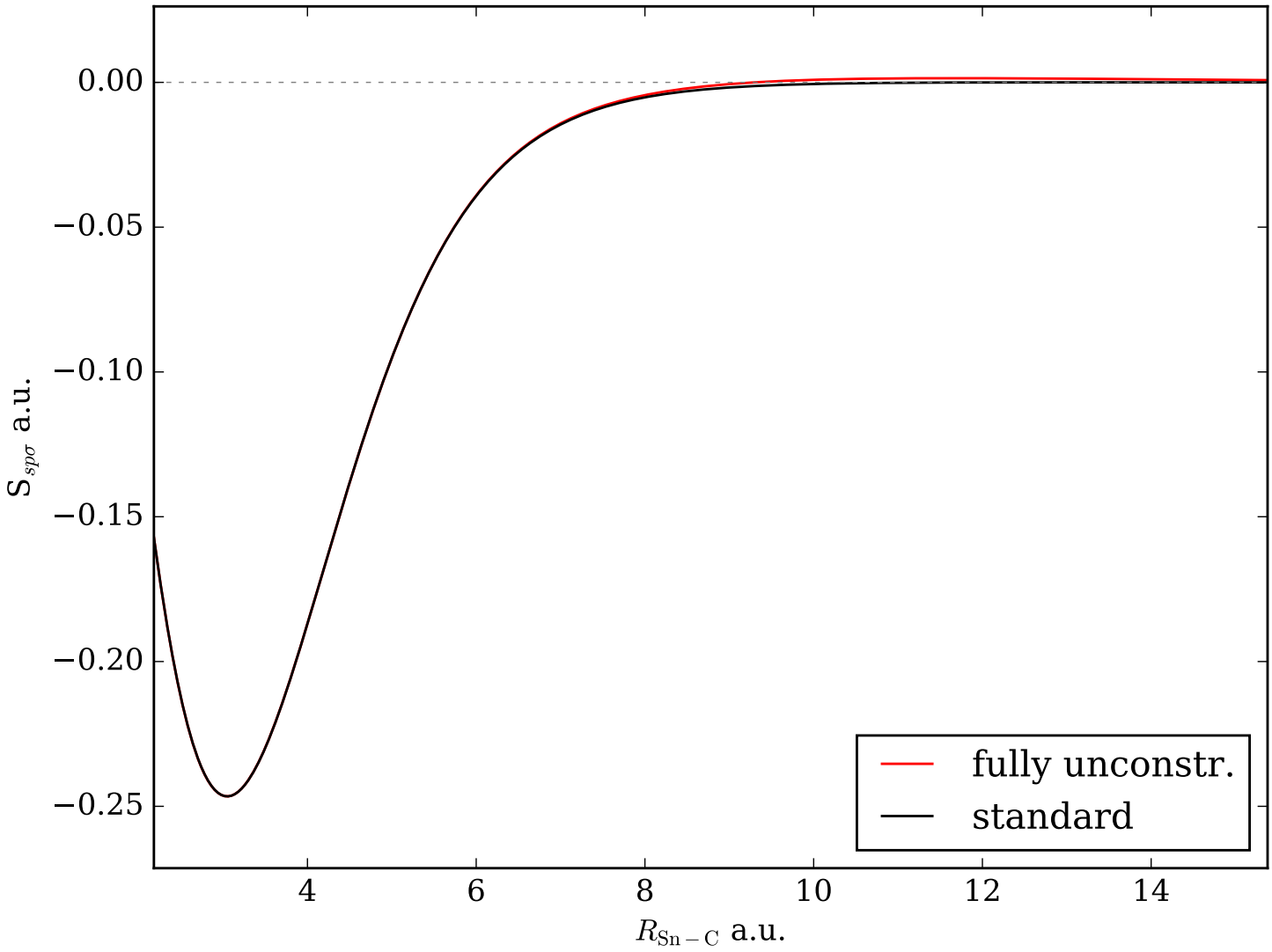

0.00
−0.05
−0.10
−0.15
−0.20
$H_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-C}}$ a.u.
fully unconstr.
standard

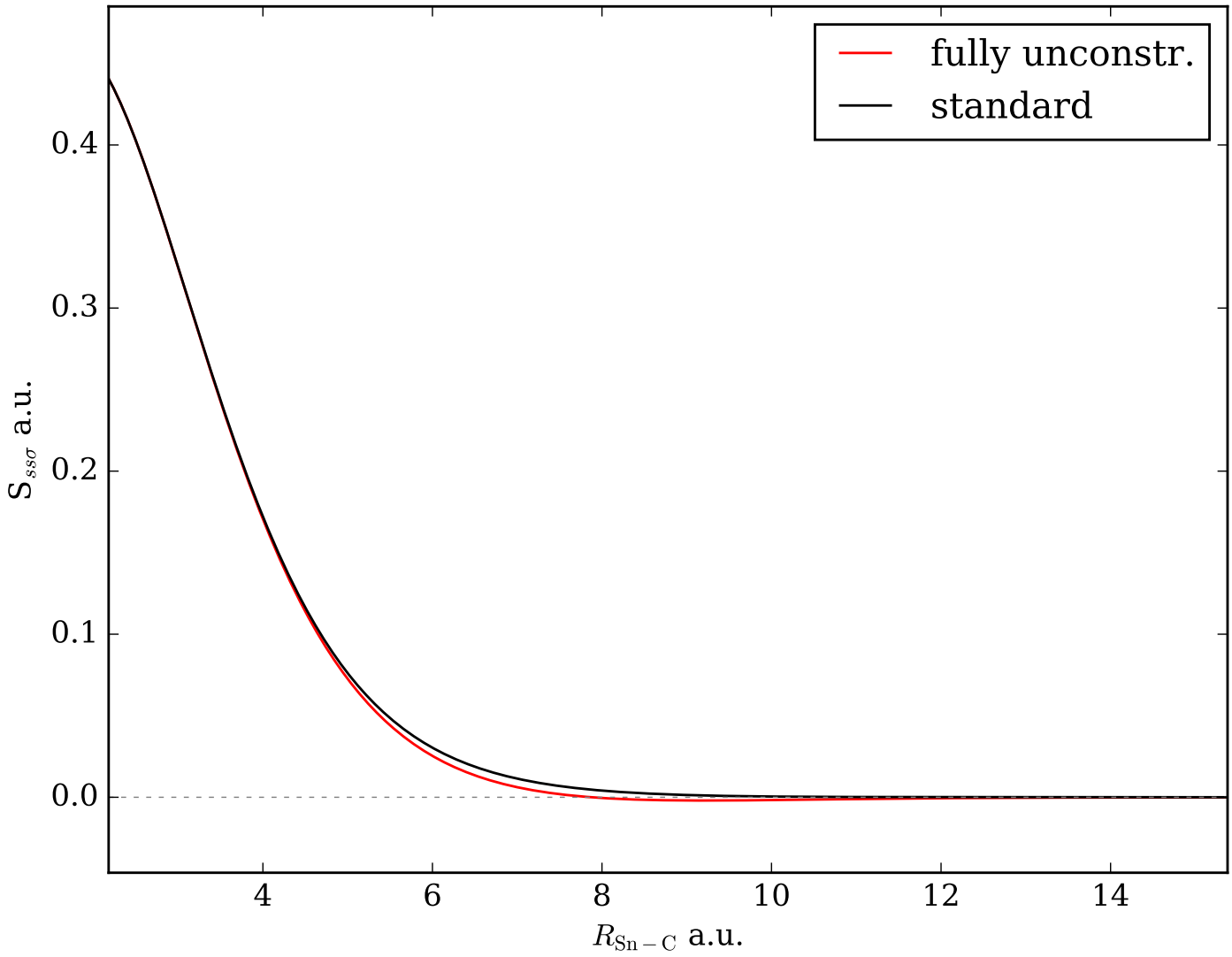

fully unconstr.
standard
0.15
0.10
0.05
0.00
$H_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-C}}$ a.u.


0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
−0.35
$H_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-C}}$ a.u.
fully unconstr.
standard


0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
$S_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-C}}$ a.u.
fully unconstr.
standard

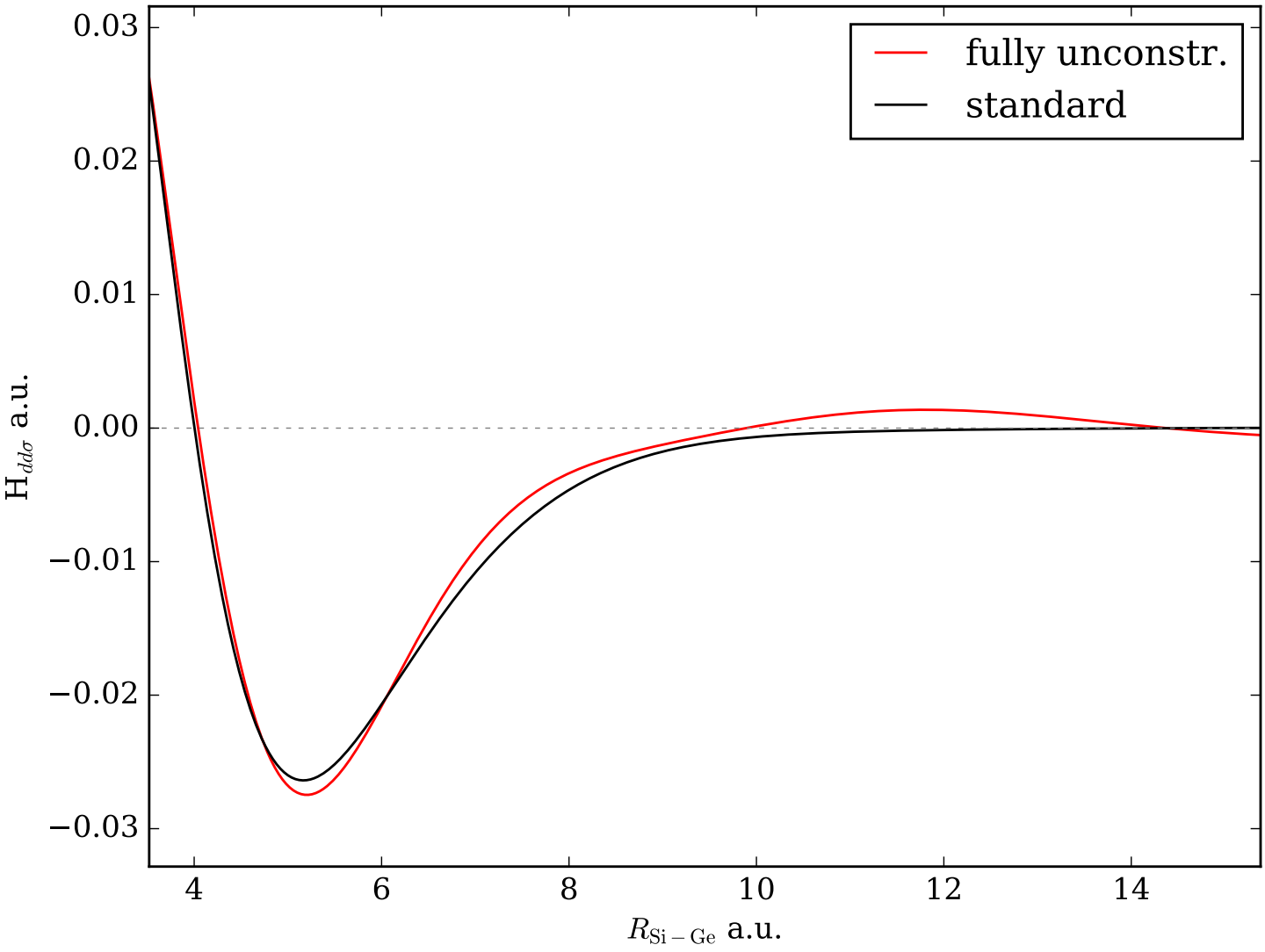

fully unconstr.
standard
0.4
0.3
0.2
0.1
0.0
$S_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-C}}$ a.u.

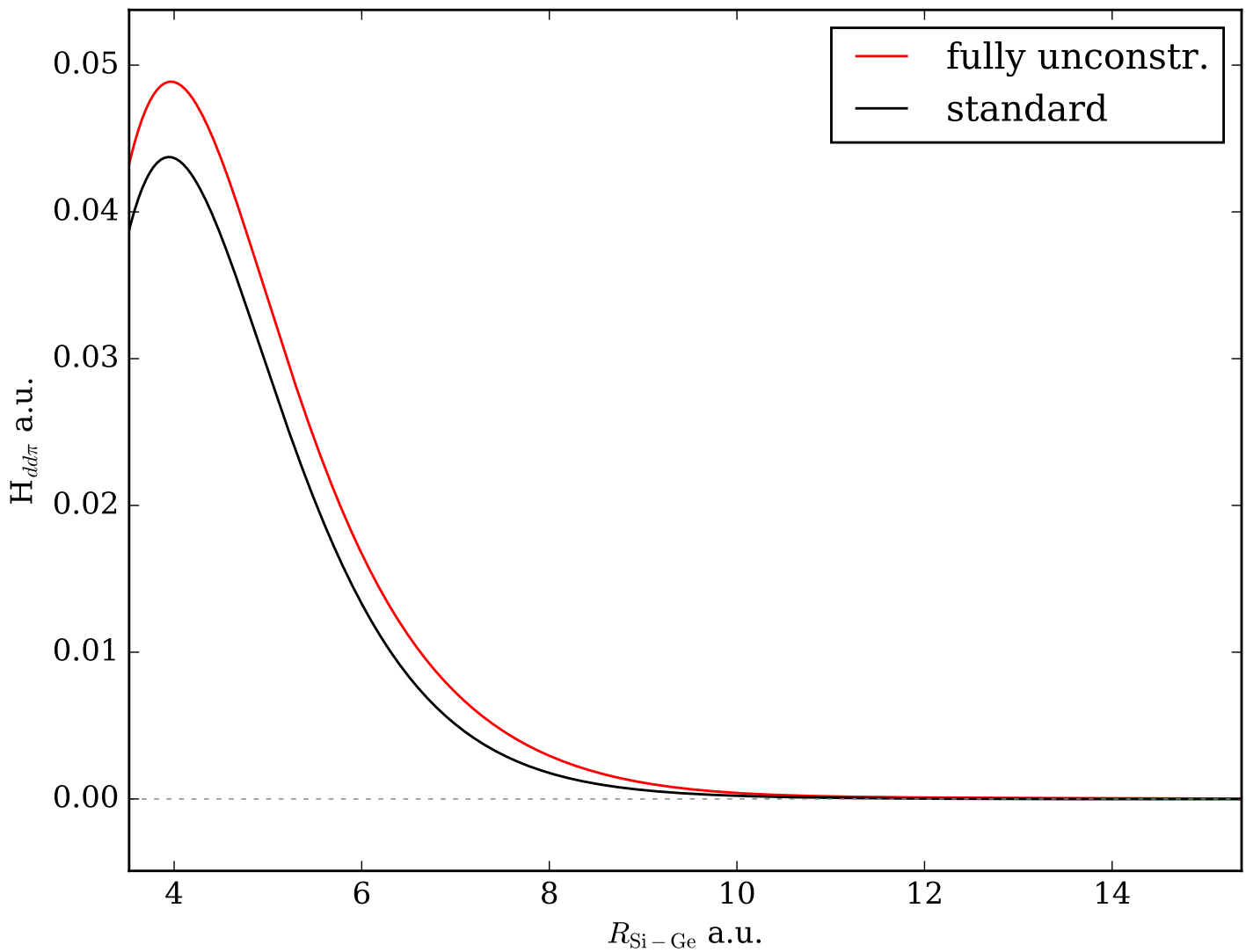

0.00
−0.05
−0.10
−0.15
−0.20
−0.25
$S_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-C}}$ a.u.
fully unconstr.
standard

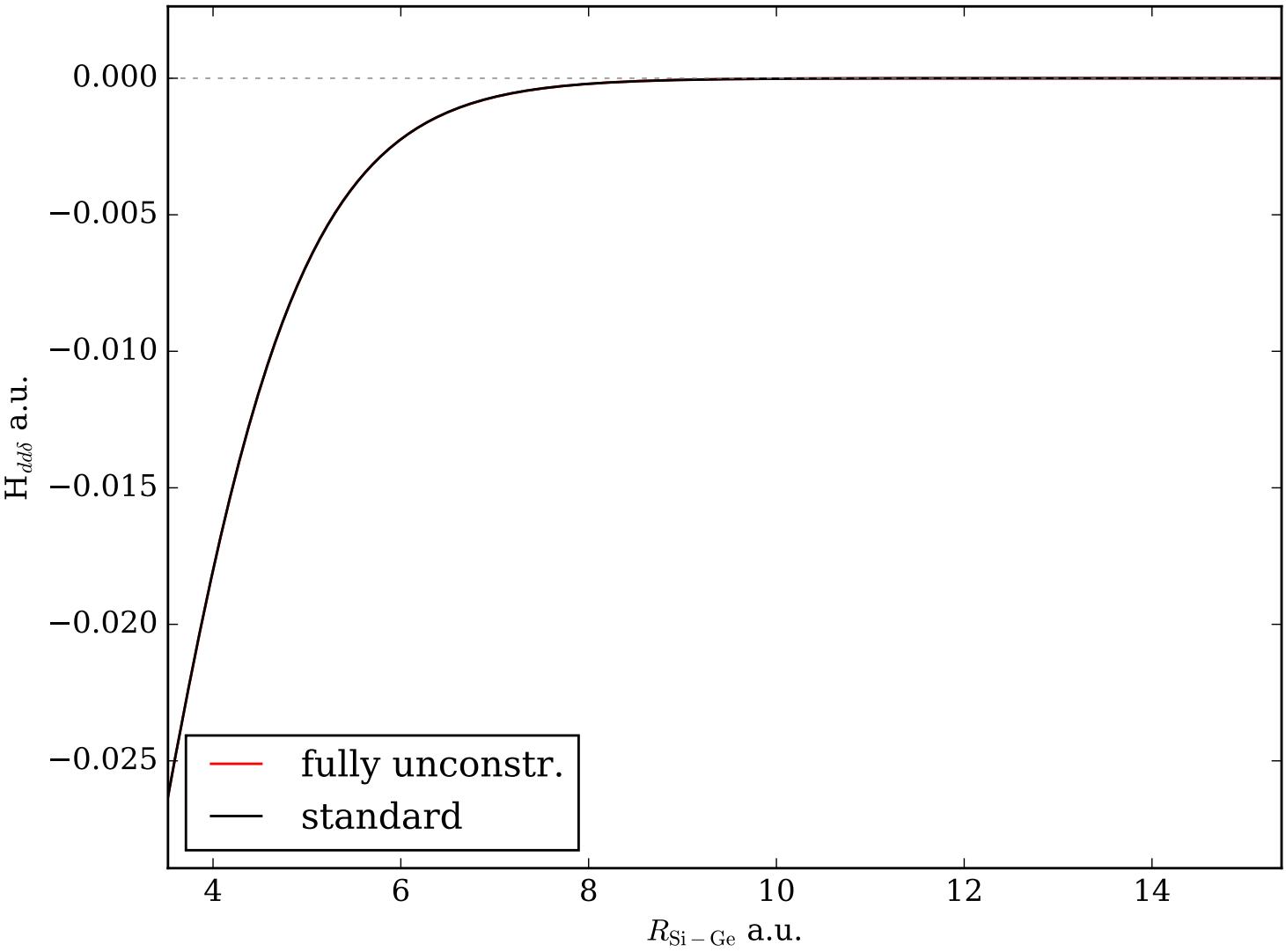

fully unconstr.
standard
0.4
0.3
0.2
0.1
0.0
$S_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-C}}$ a.u.

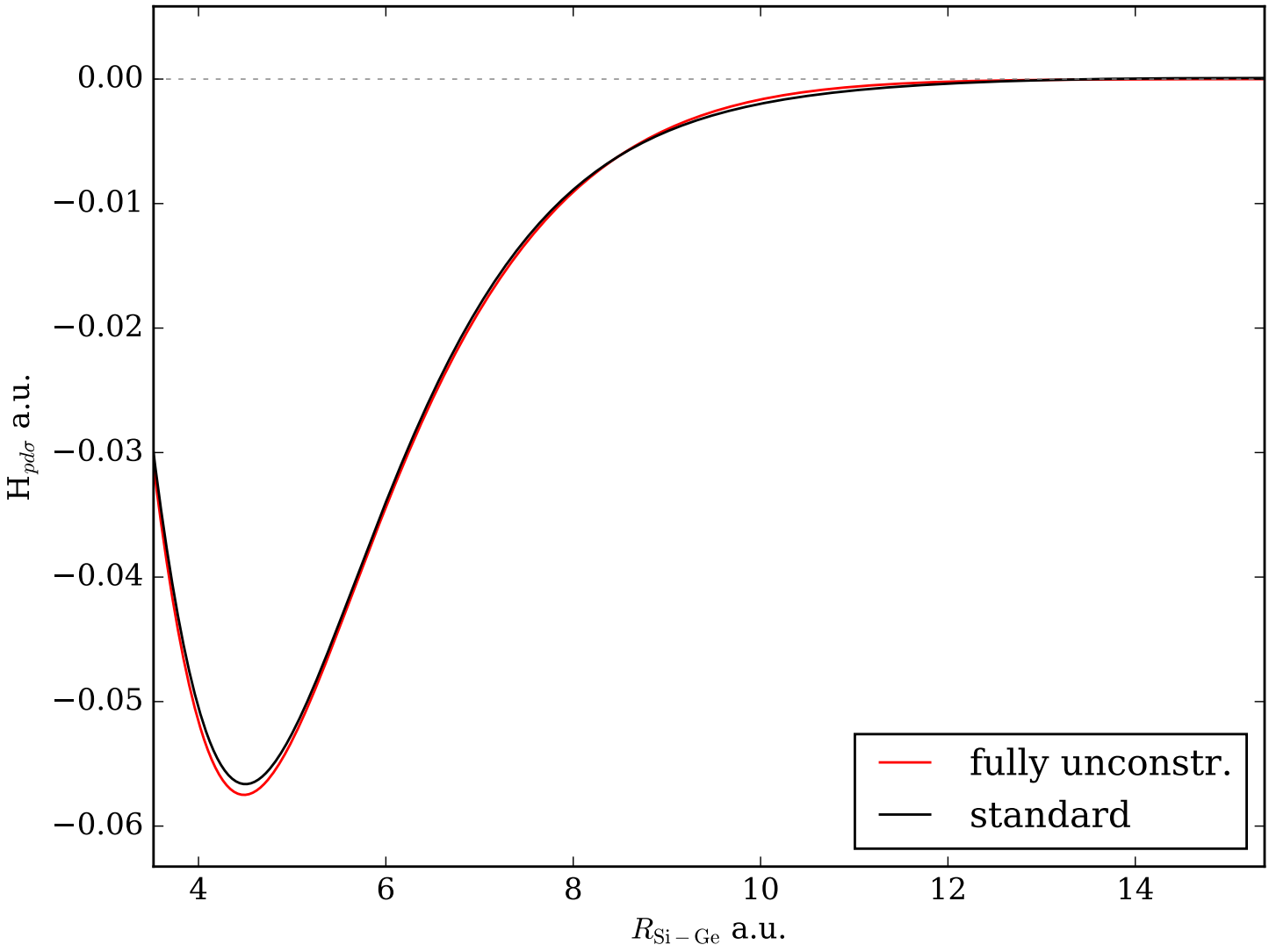
11 Si-Ge

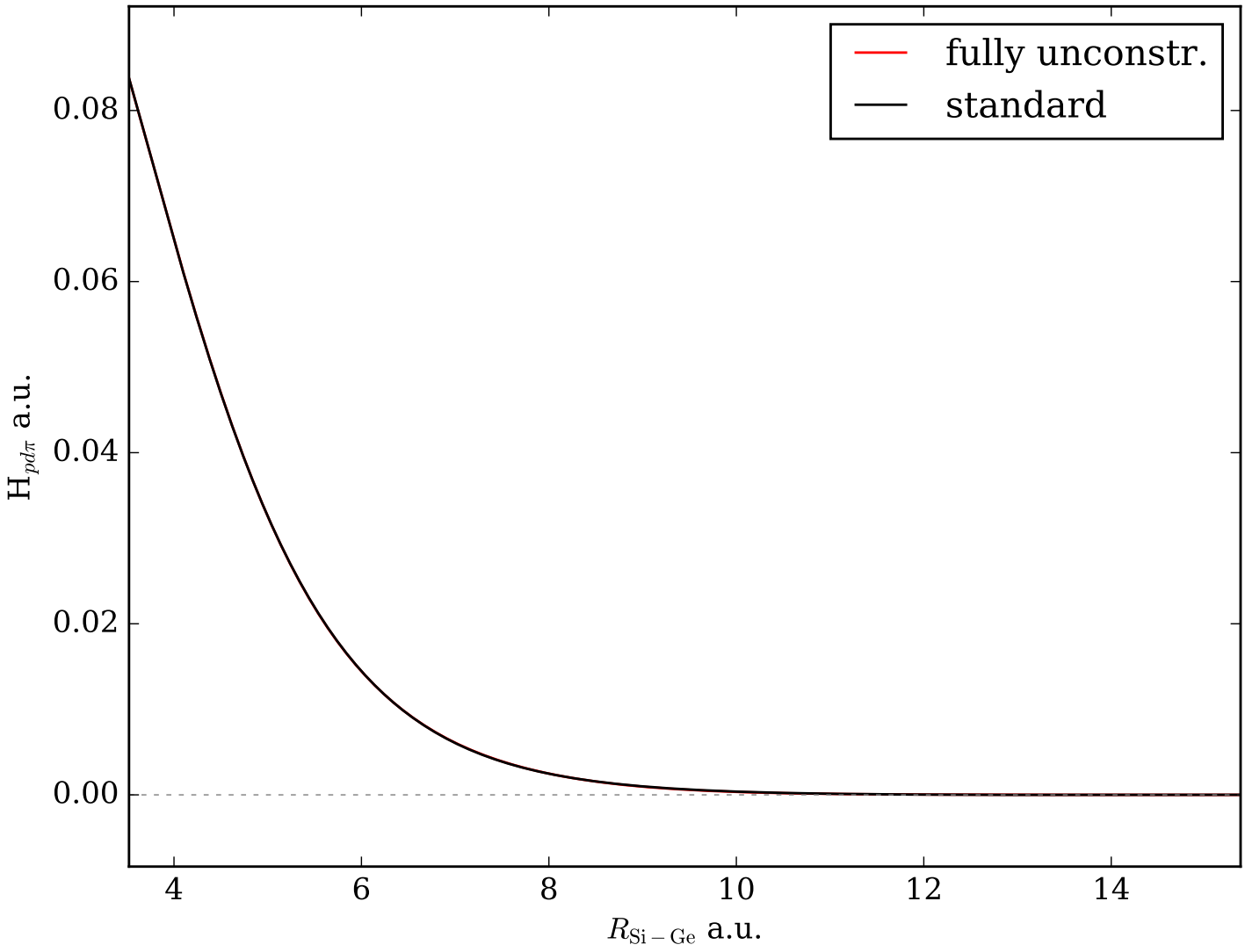
11.1 Electronic

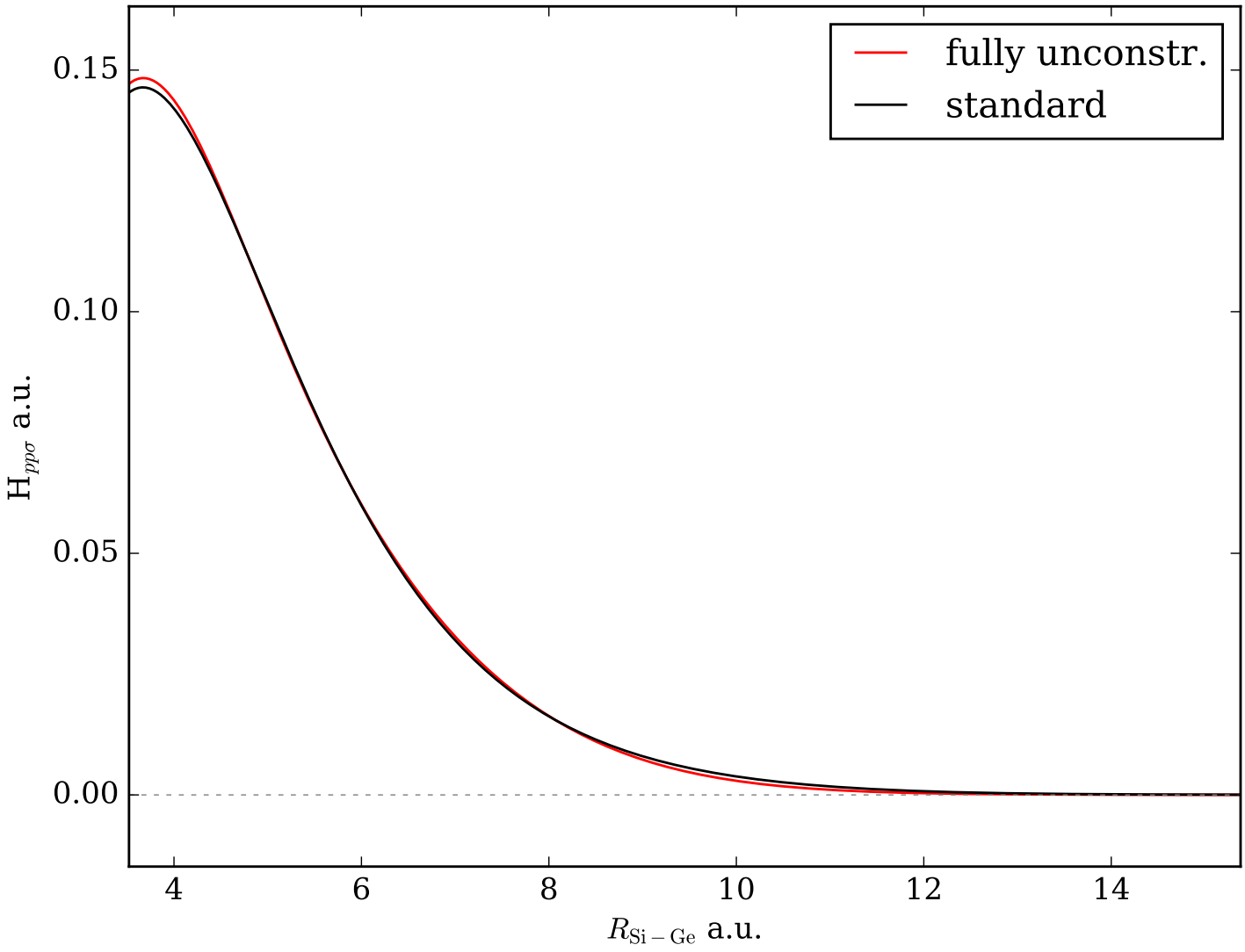


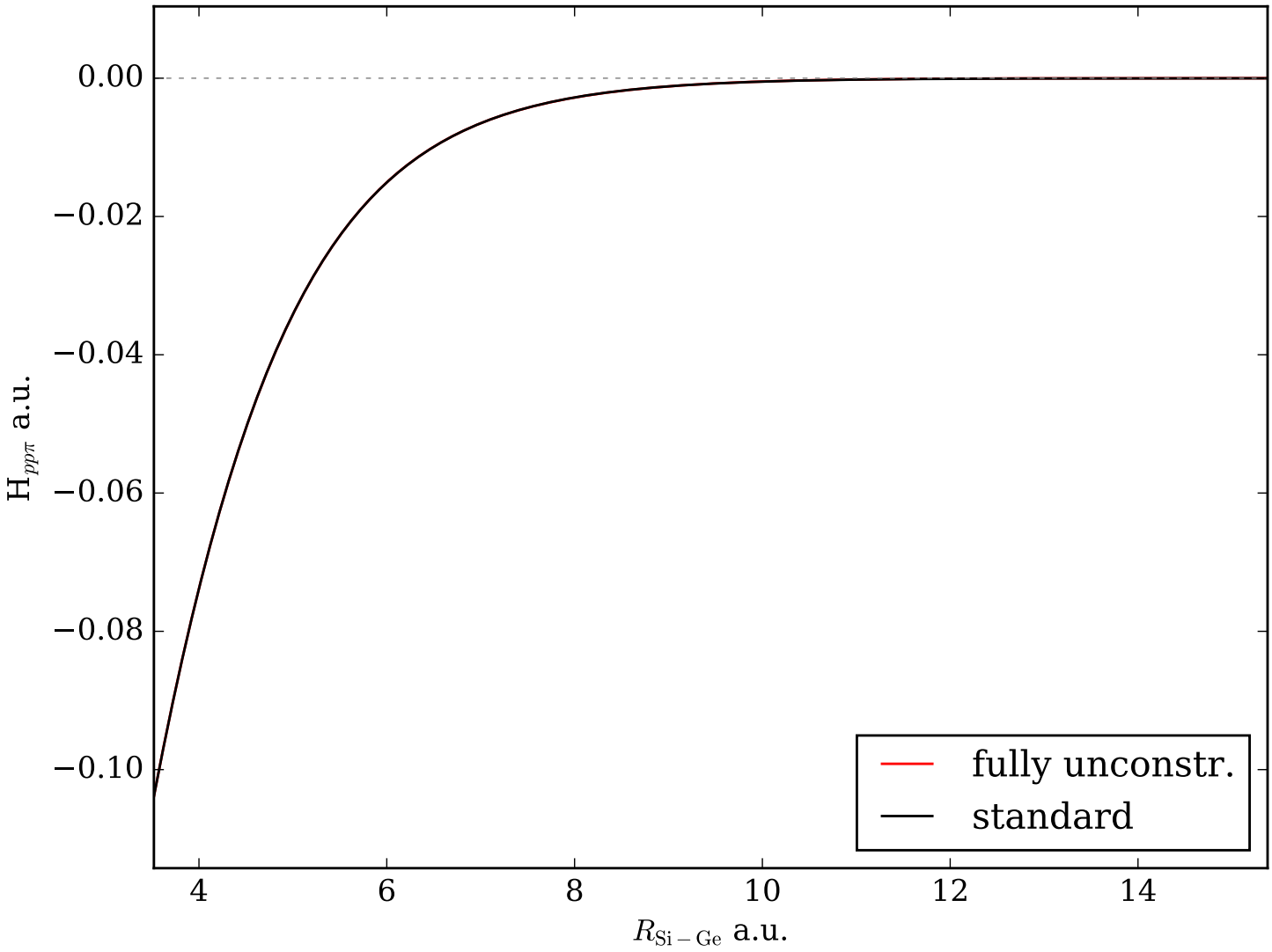

fully unconstr.
standard
0.05
0.04
0.03
0.02
0.01
0.00
$H_{dd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.

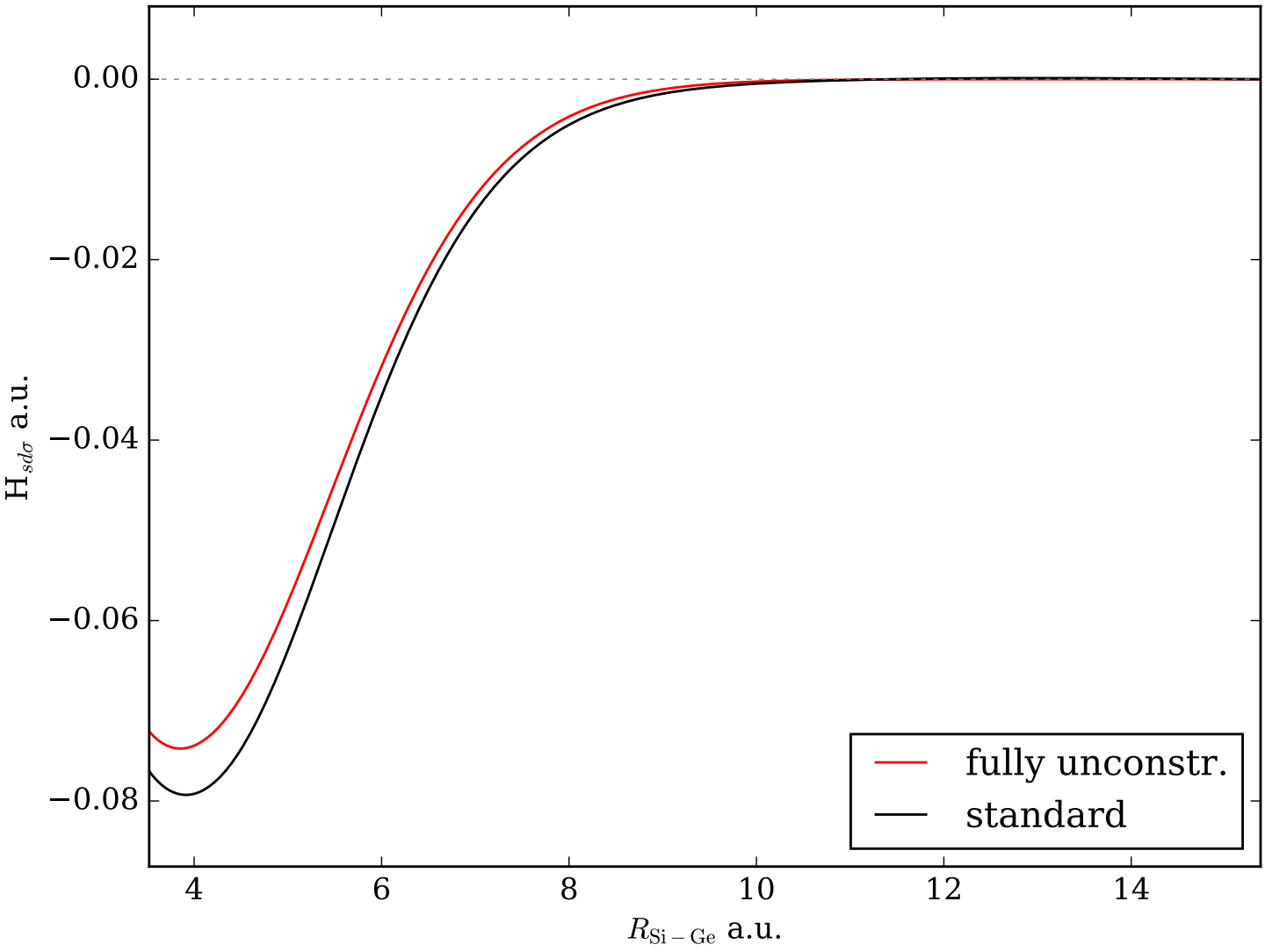

0.000
−0.005
−0.010
−0.015
−0.020
−0.025
$H_{dd\delta}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.
fully unconstr.
standard

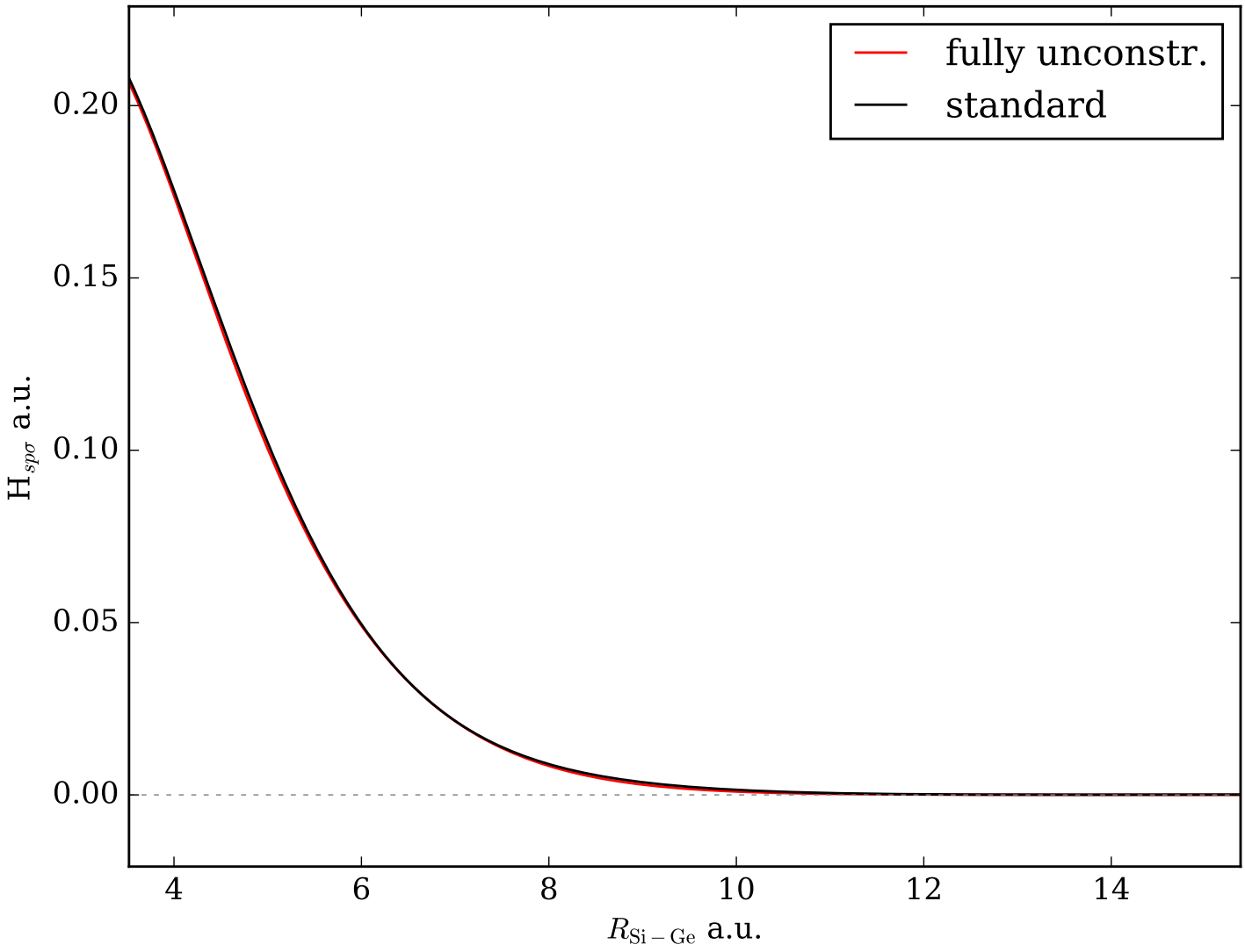

0.00
−0.01
−0.02
−0.03
−0.04
−0.05
−0.06
$H_{pd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.
fully unconstr.
standard

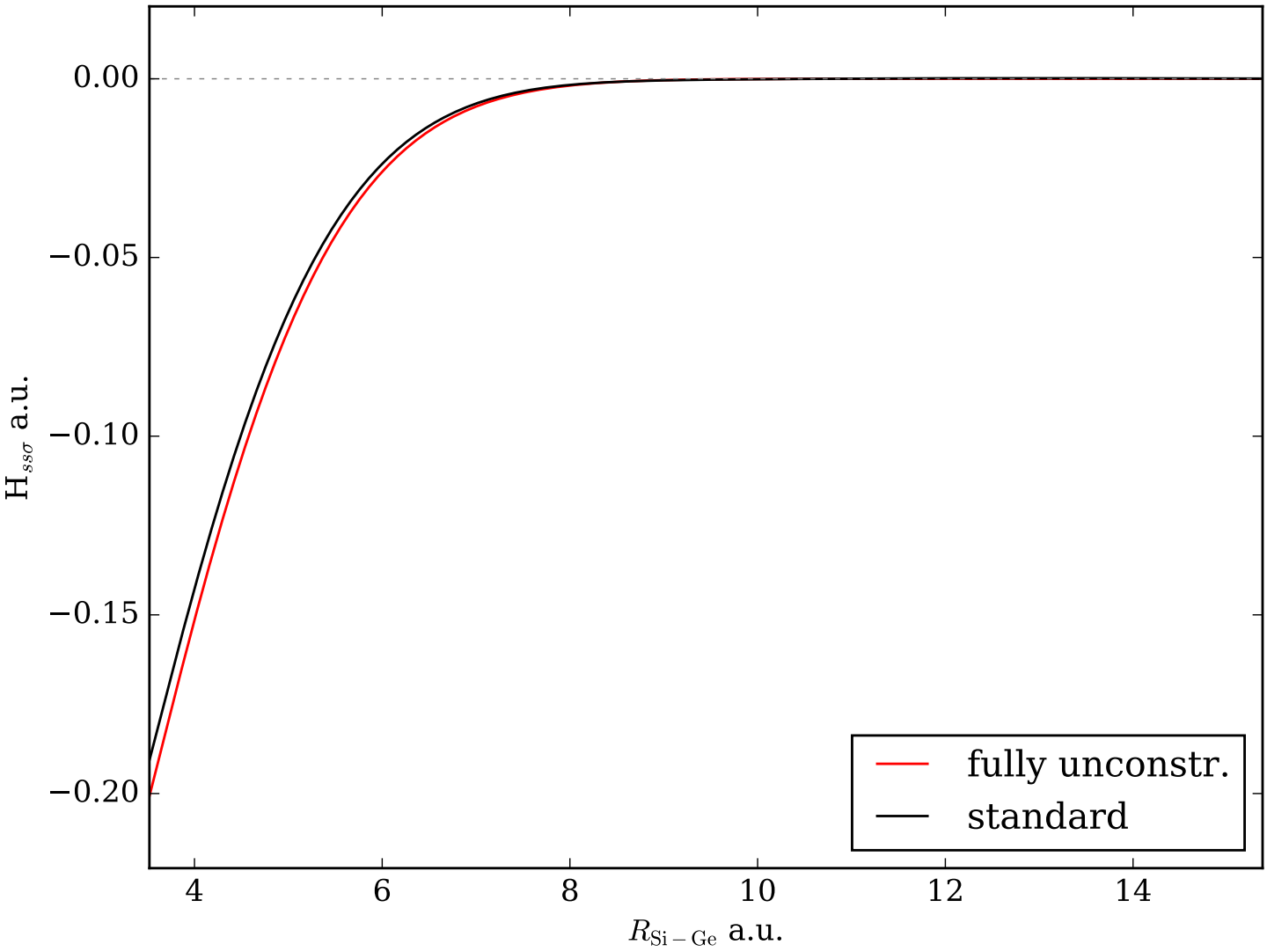

fully unconstr.
standard
0.08
0.06
0.04
0.02
0.00
$H_{pd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.


fully unconstr.
standard
0.15
0.10
0.05
0.00
$H_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.


0.00
−0.02
−0.04
−0.06
−0.08
−0.10
$H_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.
fully unconstr.
standard


0.00
−0.02
−0.04
−0.06
−0.08
$H_{sd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.20
0.15
0.10
0.05
0.00
$H_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.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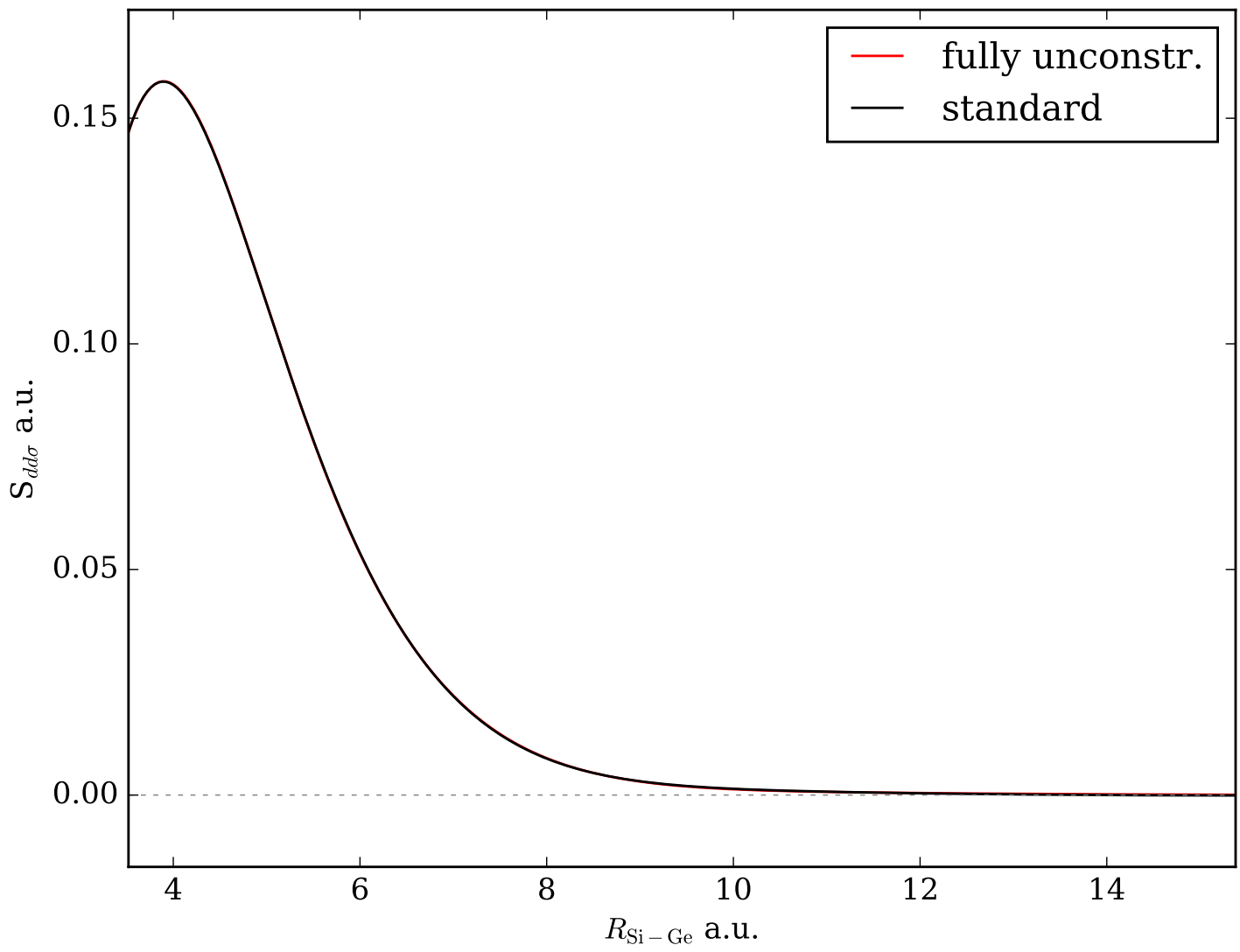
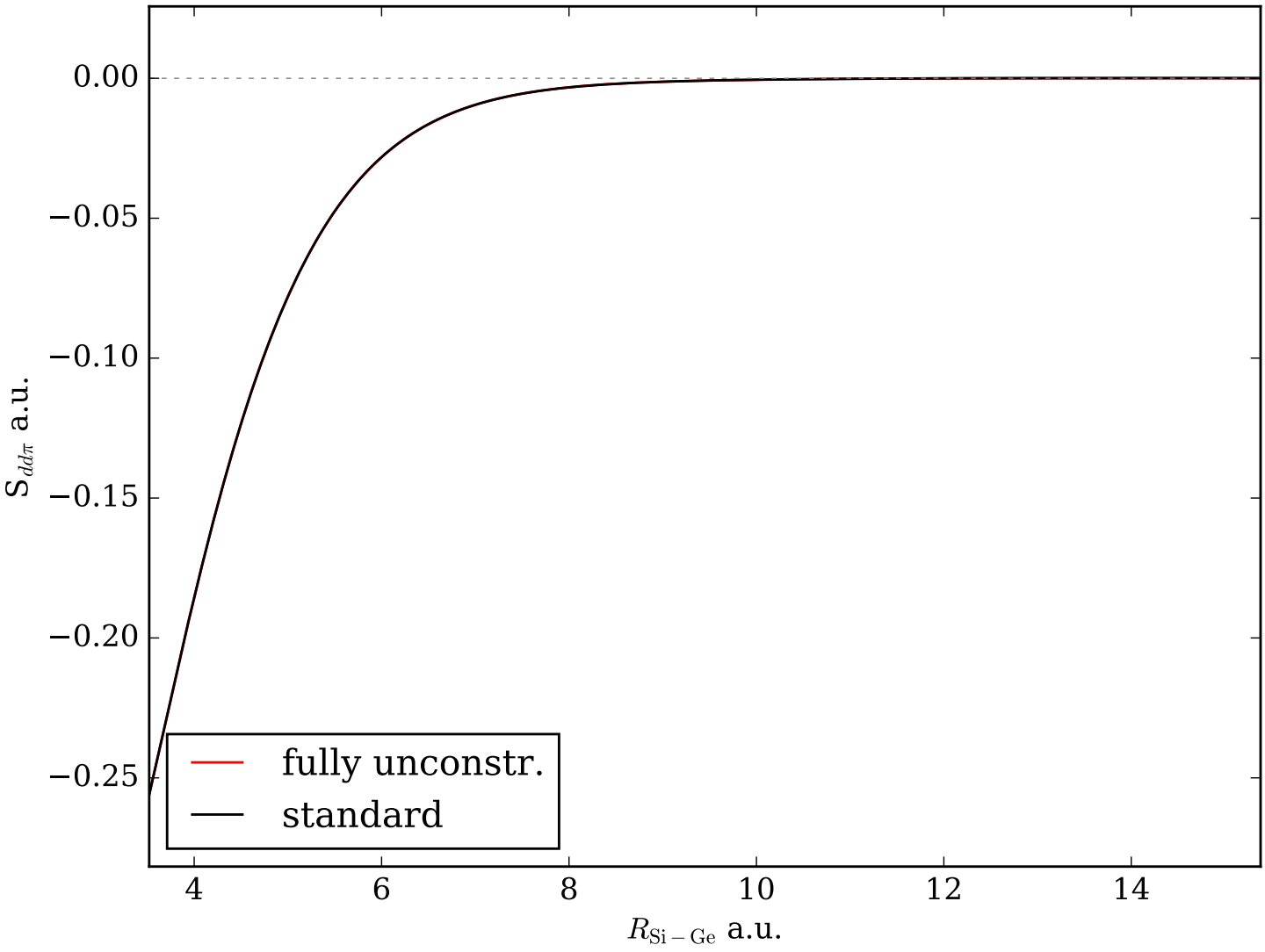
−0.05
−0.10
−0.15
−0.20
$H_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.15
0.10
0.05
0.00
$S_{dd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.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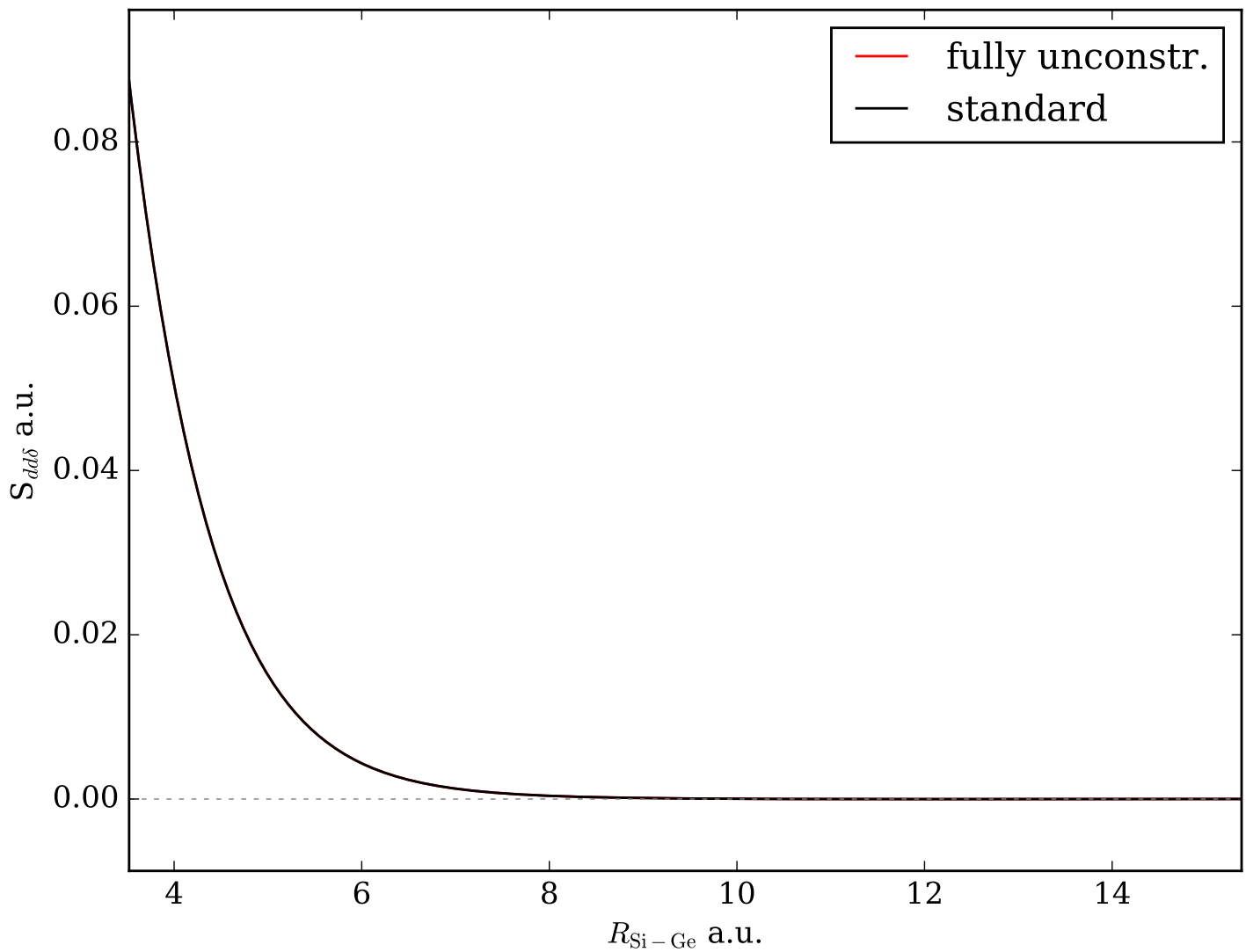
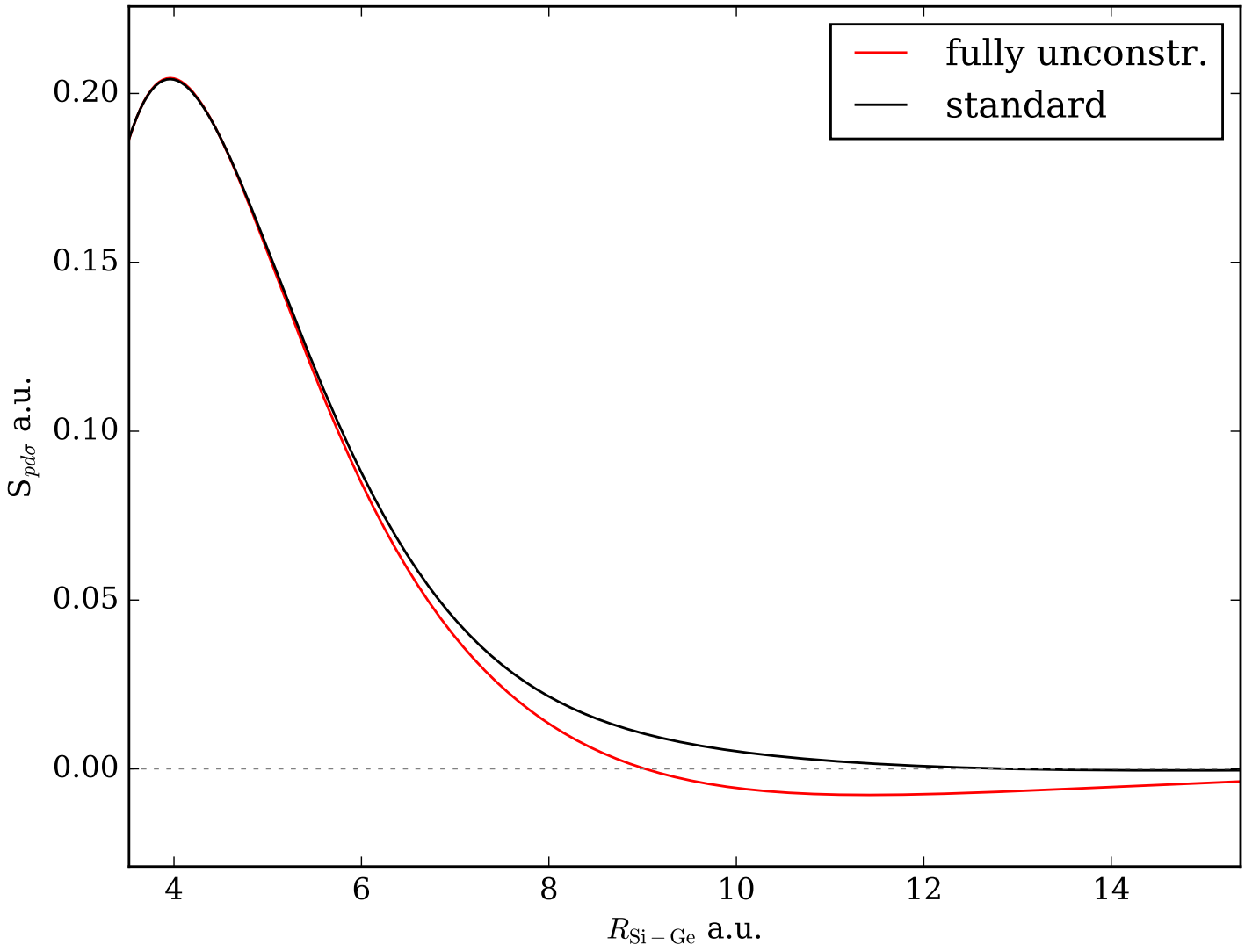
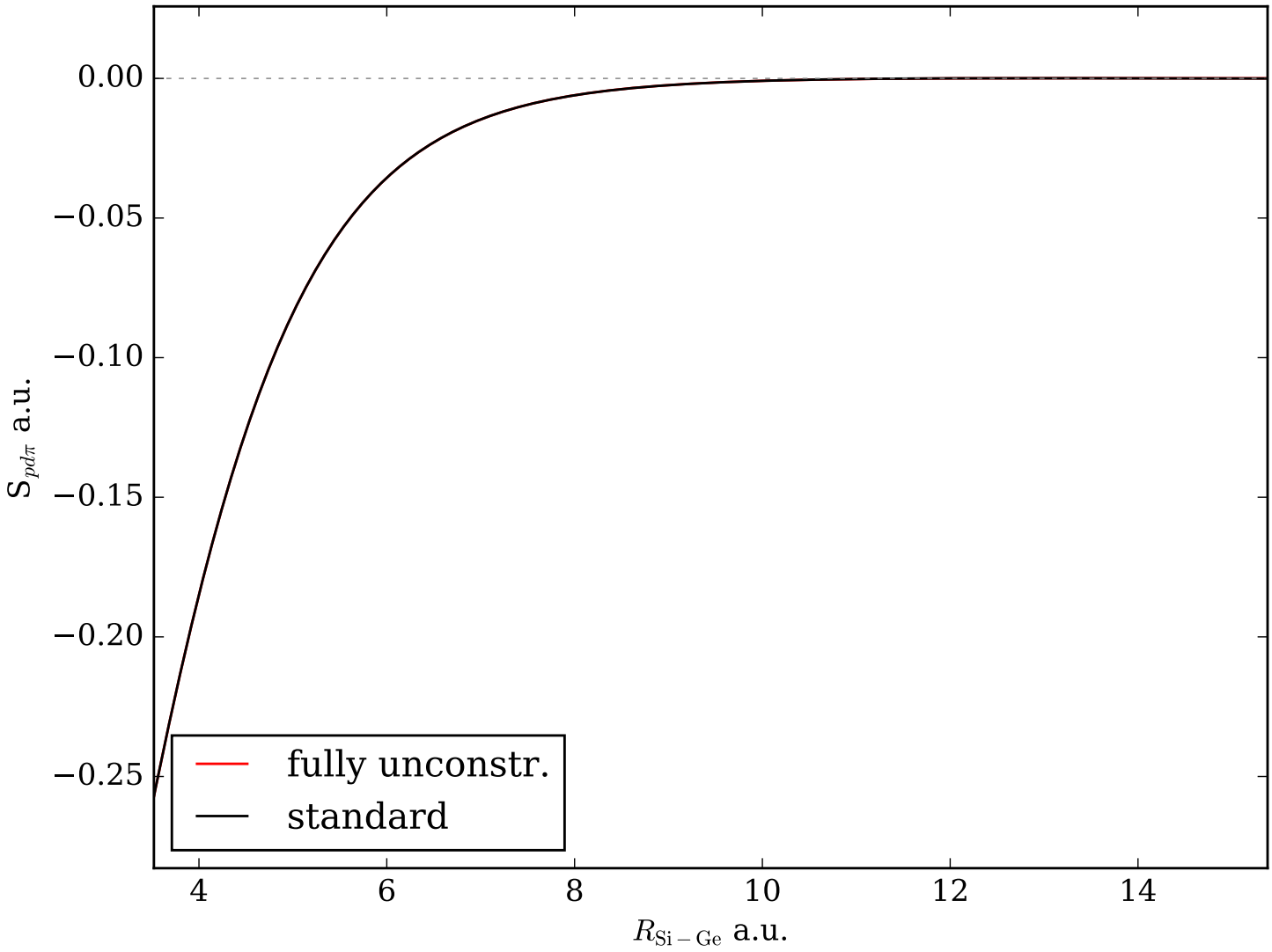
−0.05
−0.10
−0.15
−0.20
−0.25
$S_{dd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.08
0.06
0.04
0.02
0.00
$S_{dd\delta}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.


fully unconstr.
standard
0.20
0.15
0.10
0.05
0.00
$S_{pd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.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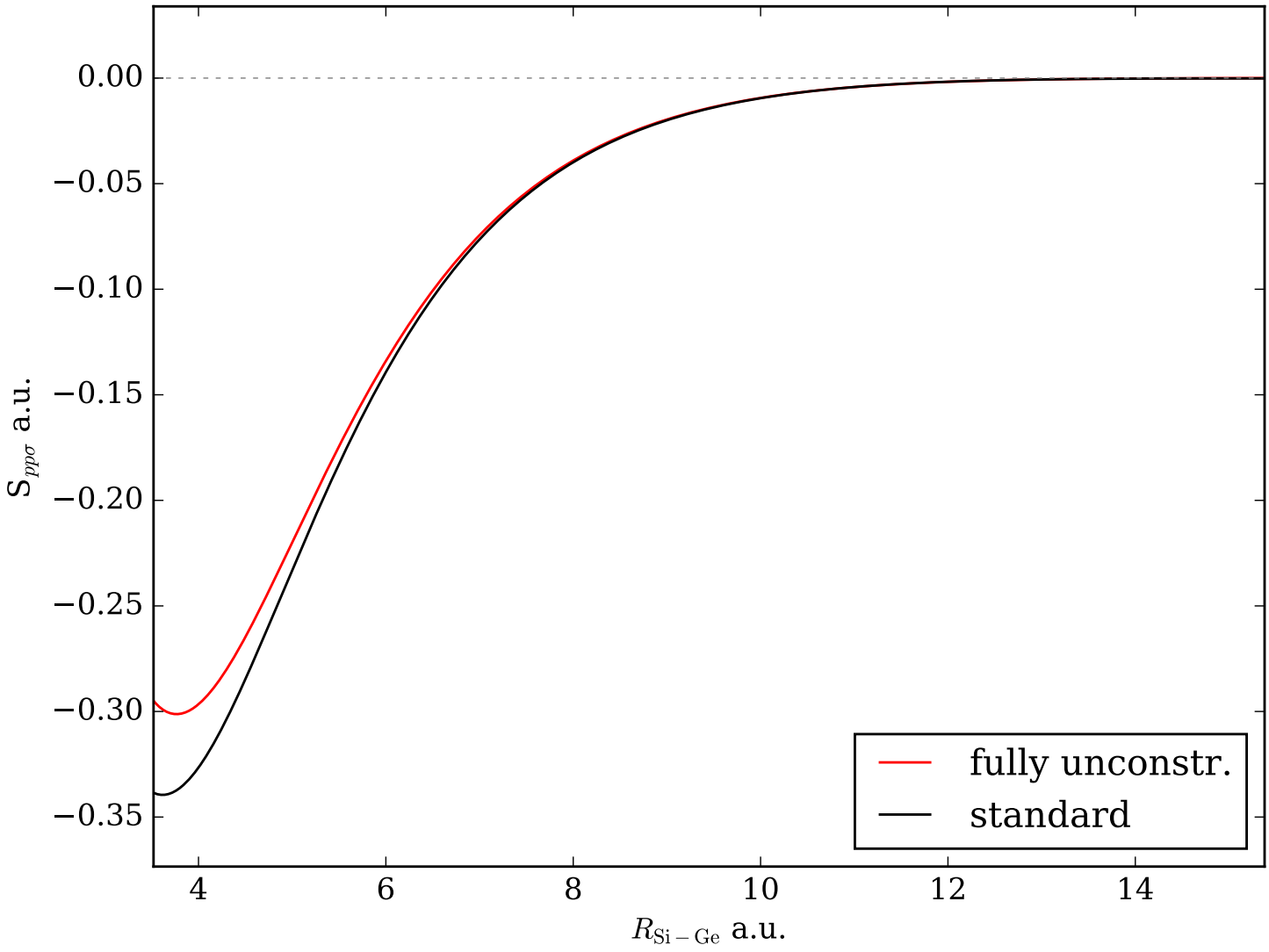
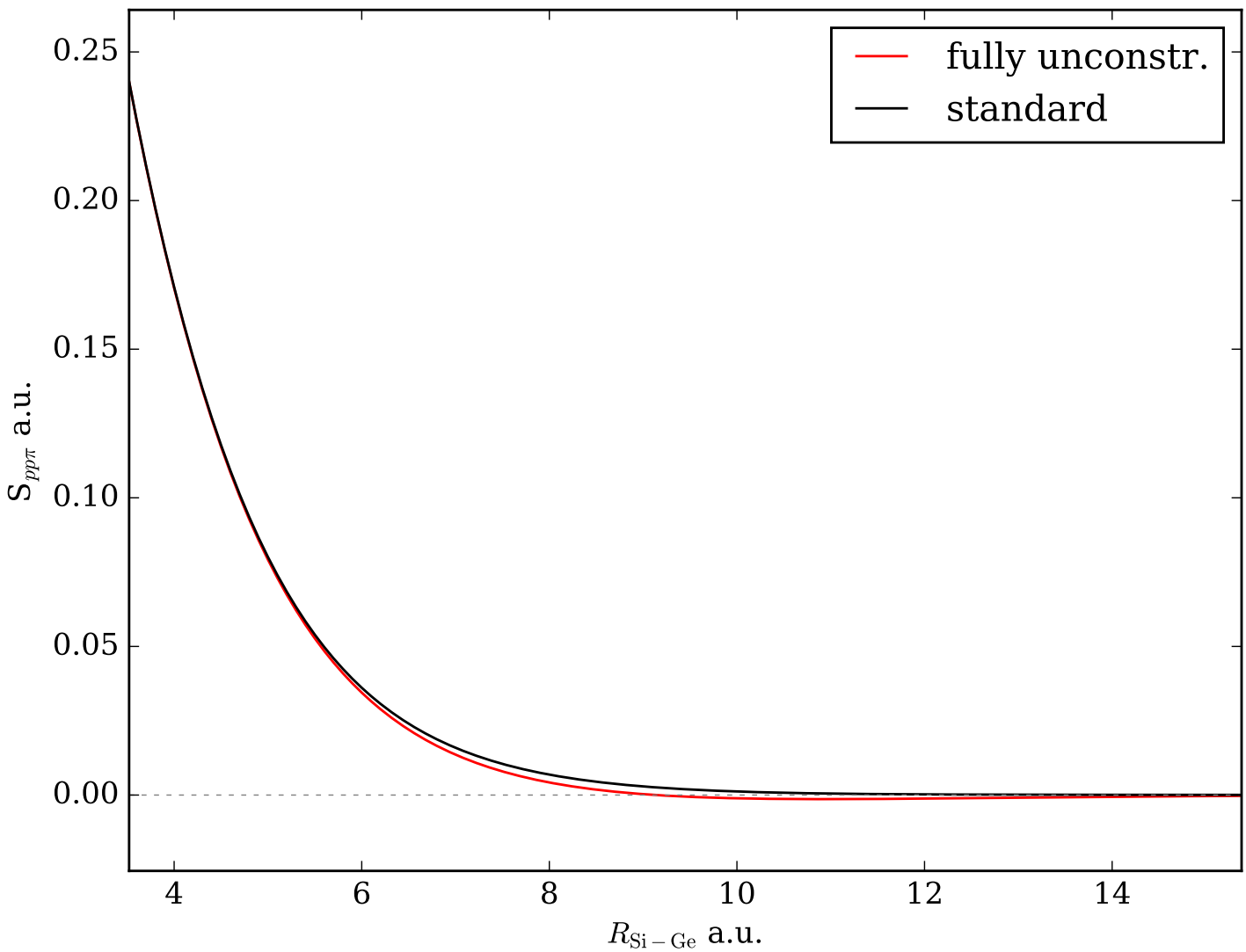
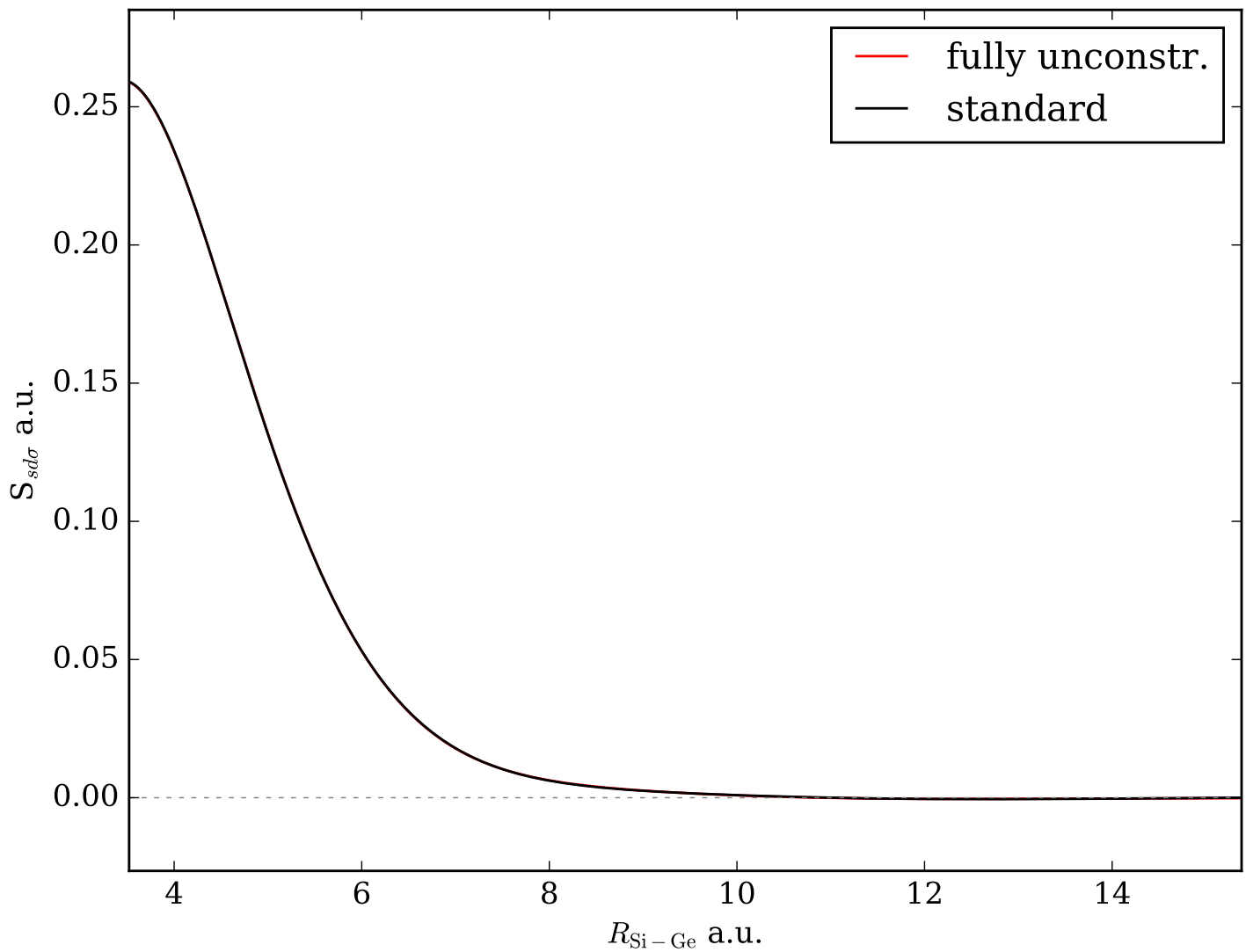
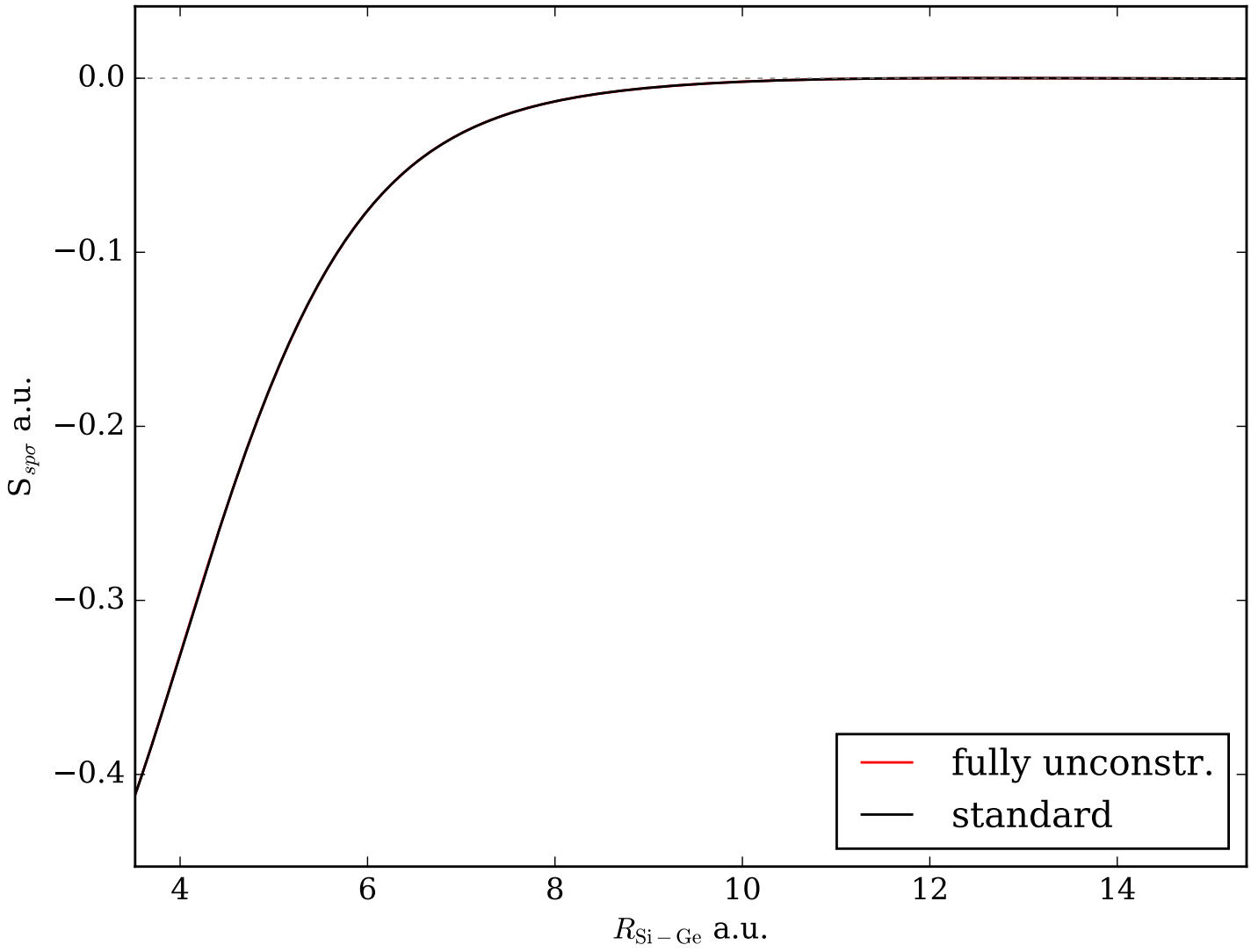
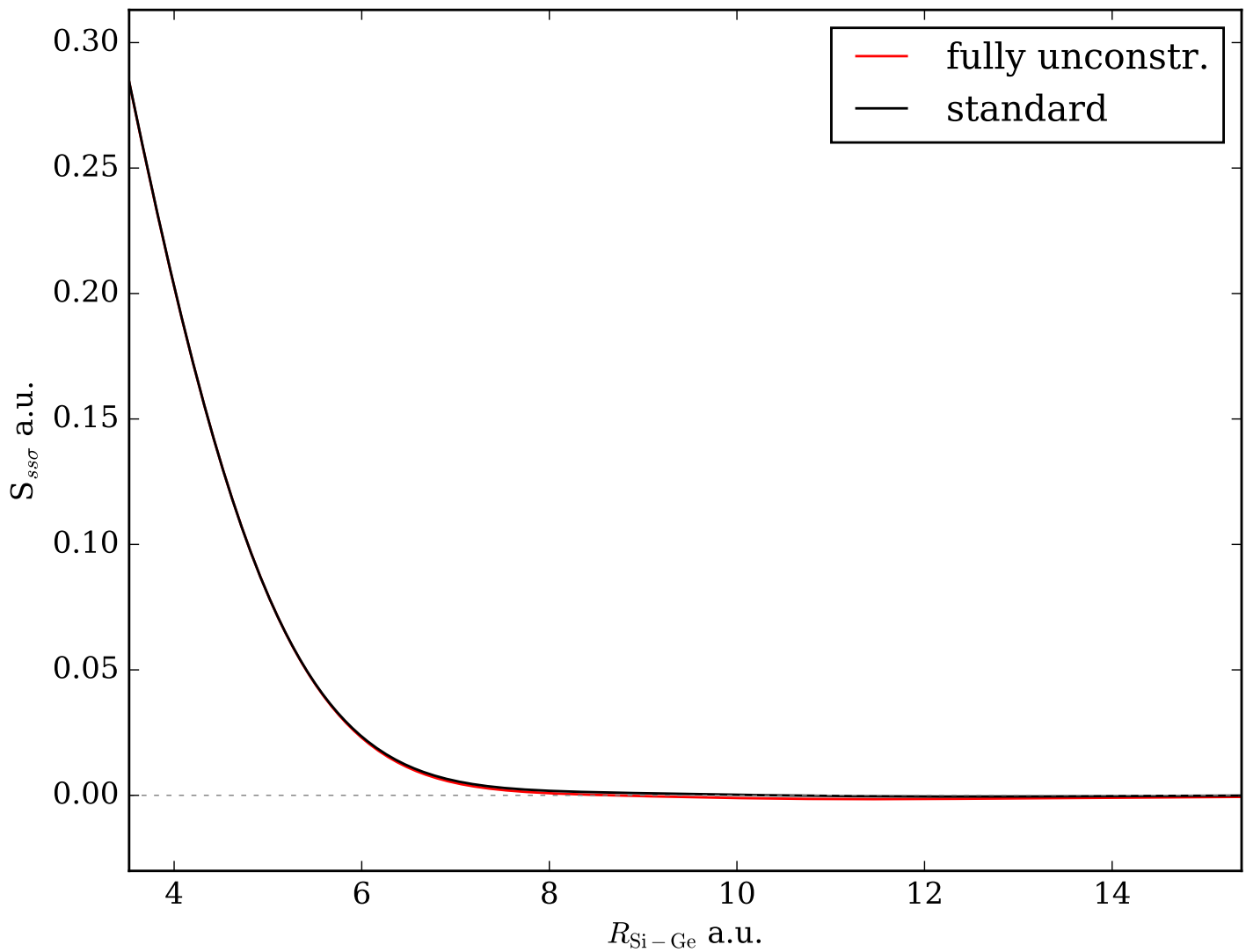
−0.05
−0.10
−0.15
−0.20
−0.25
$S_{pd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.
fully unconstr.
standard


0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
−0.35
$S_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.
fully unconstr.
standard

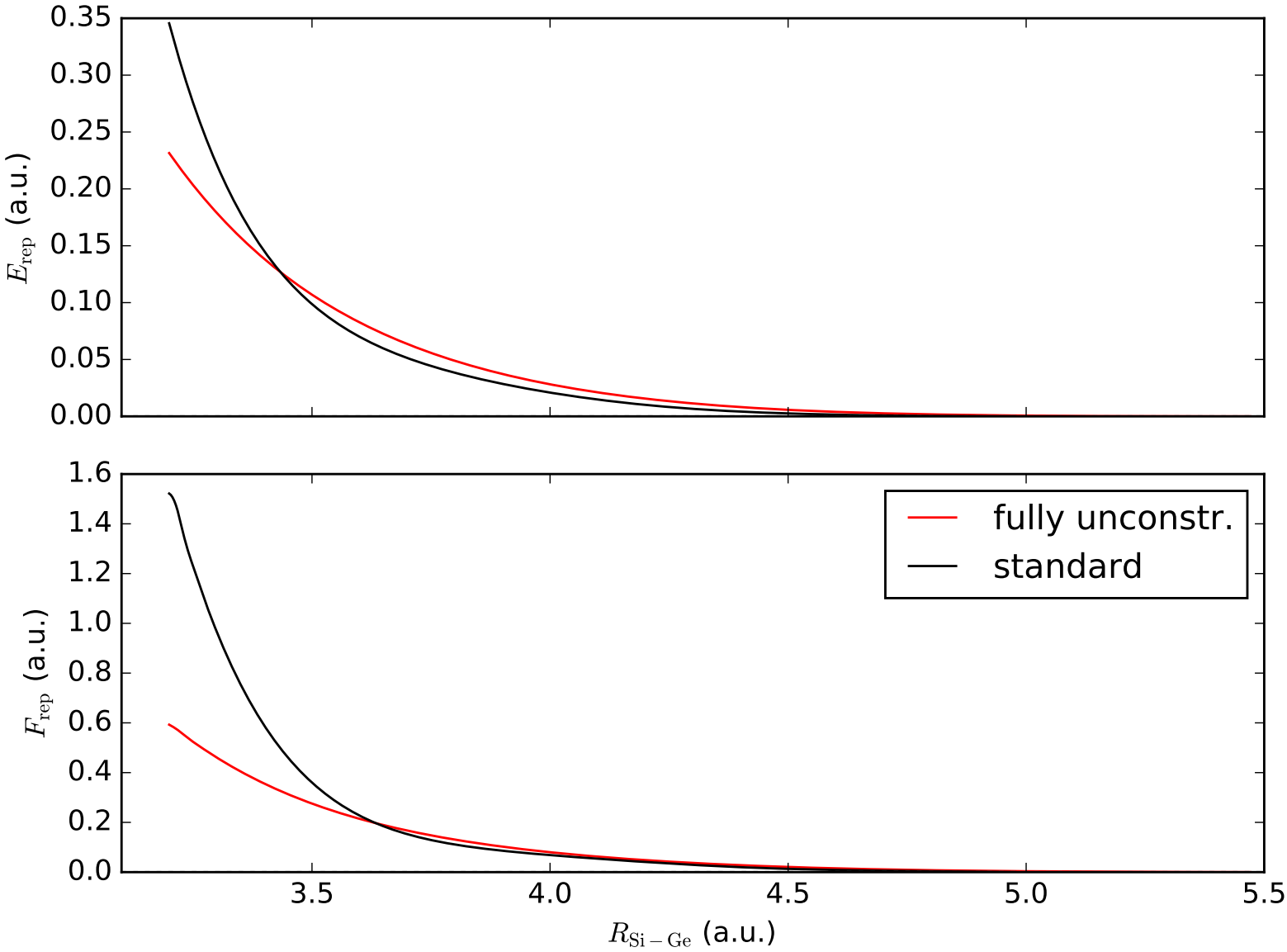

fully unconstr.
standard
0.25
0.20
0.15
0.10
0.05
0.00
$S_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.


fully unconstr.
standard
0.25
0.20
0.15
0.10
0.05
0.00
$S_{sd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.


0.0
−0.1
−0.2
−0.3
−0.4
$S_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.
fully unconstr.
standard

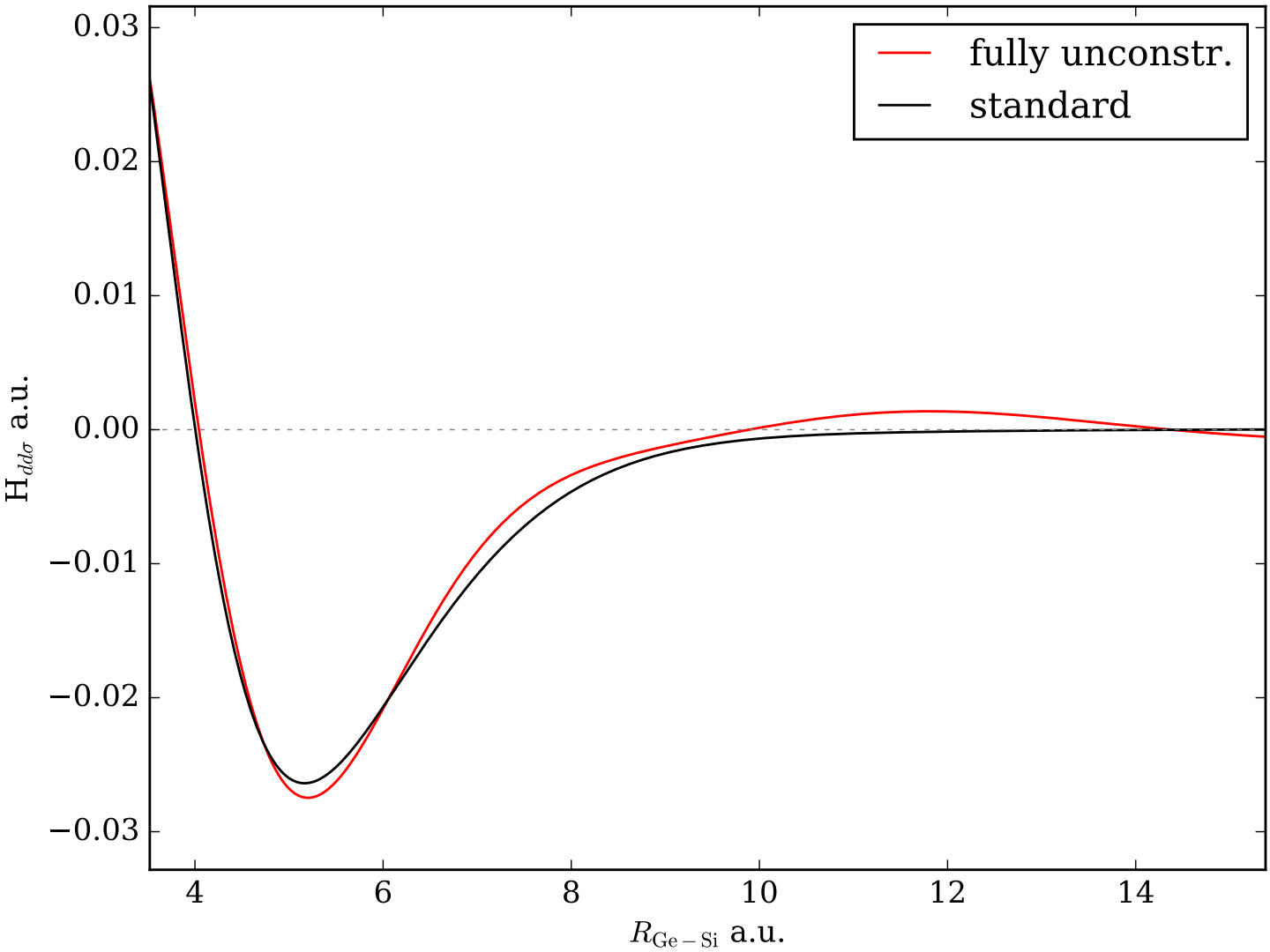

fully unconstr.
standard
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$S_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Ge}}$ a.u.

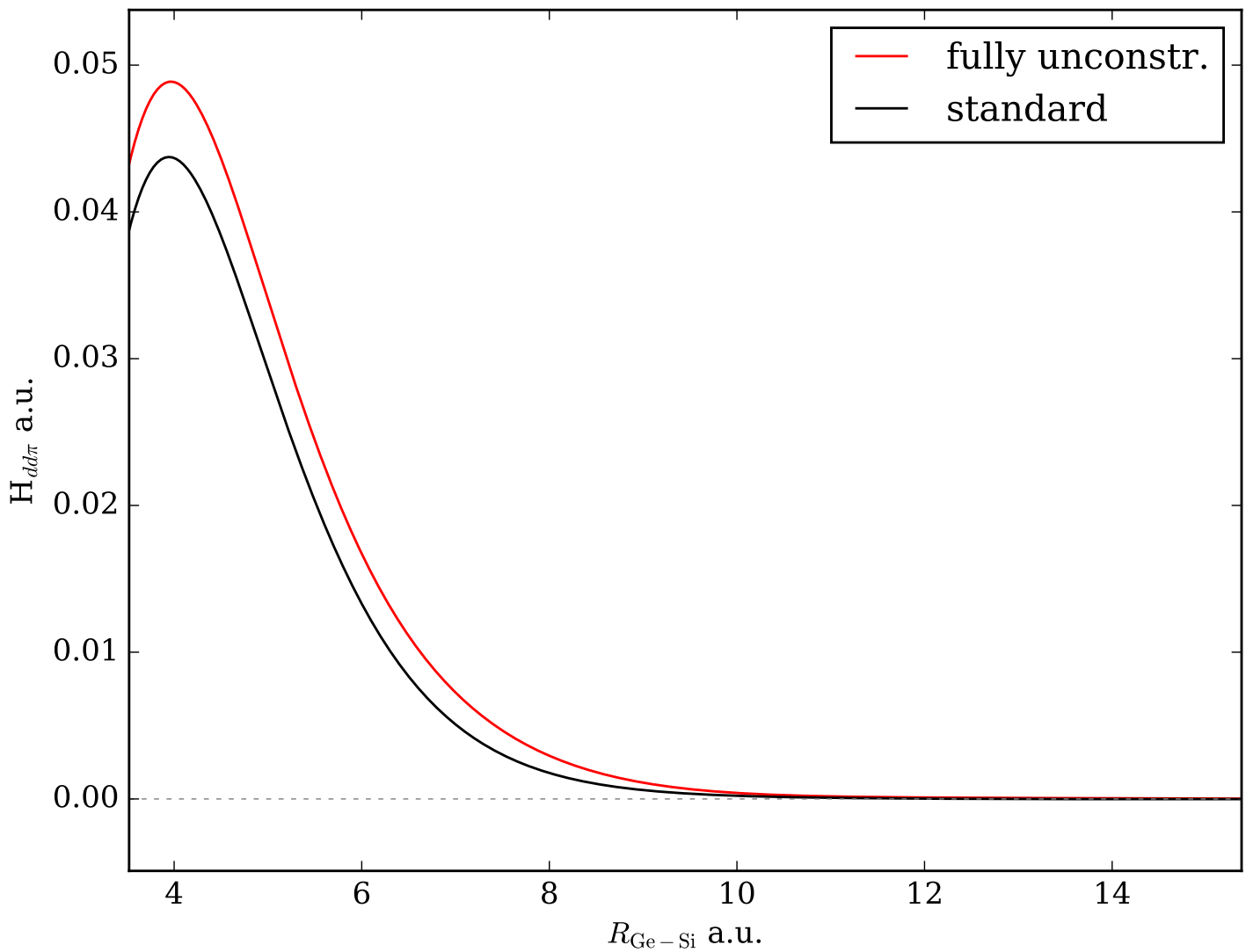
11.2 Repulsive

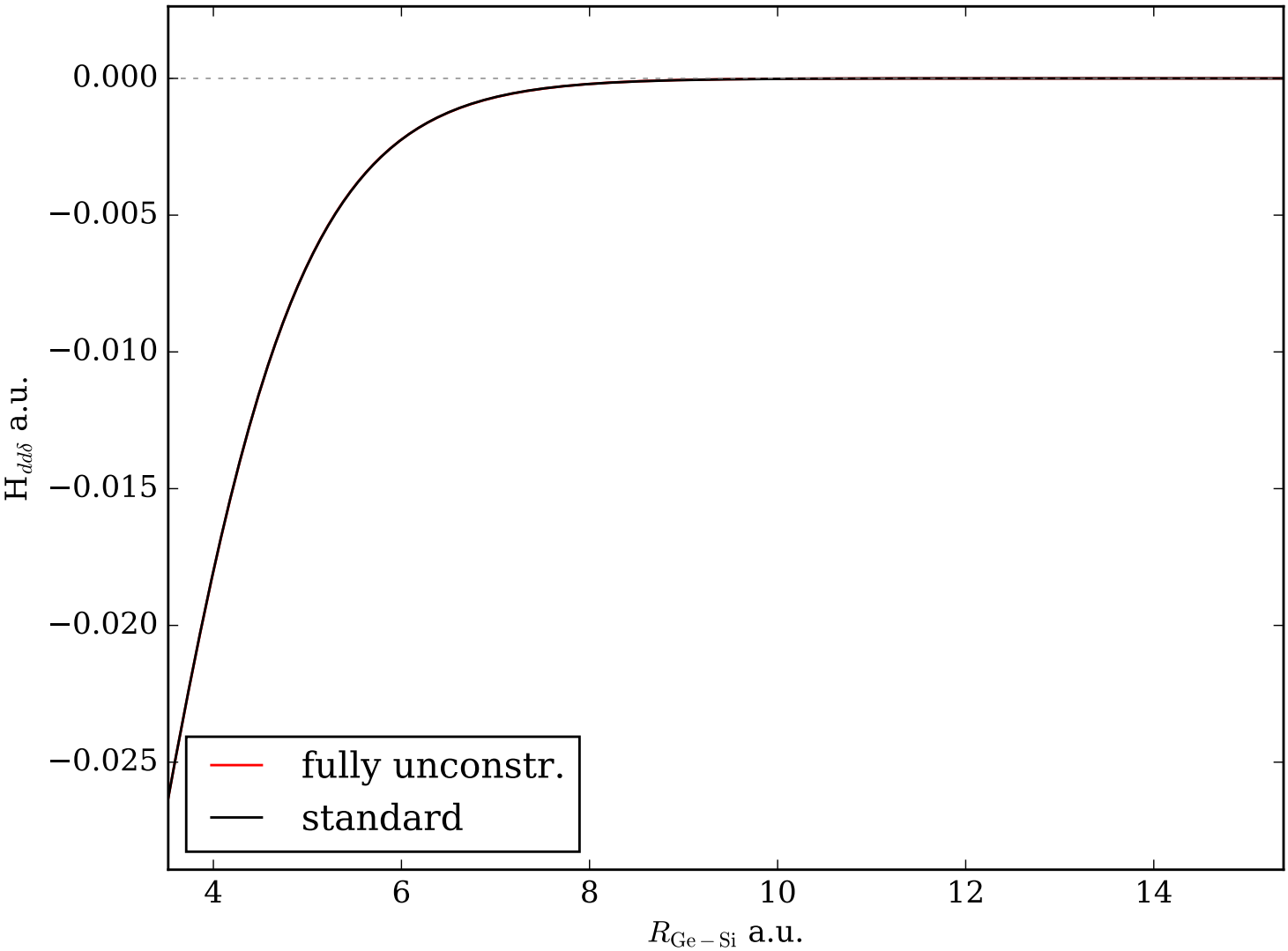


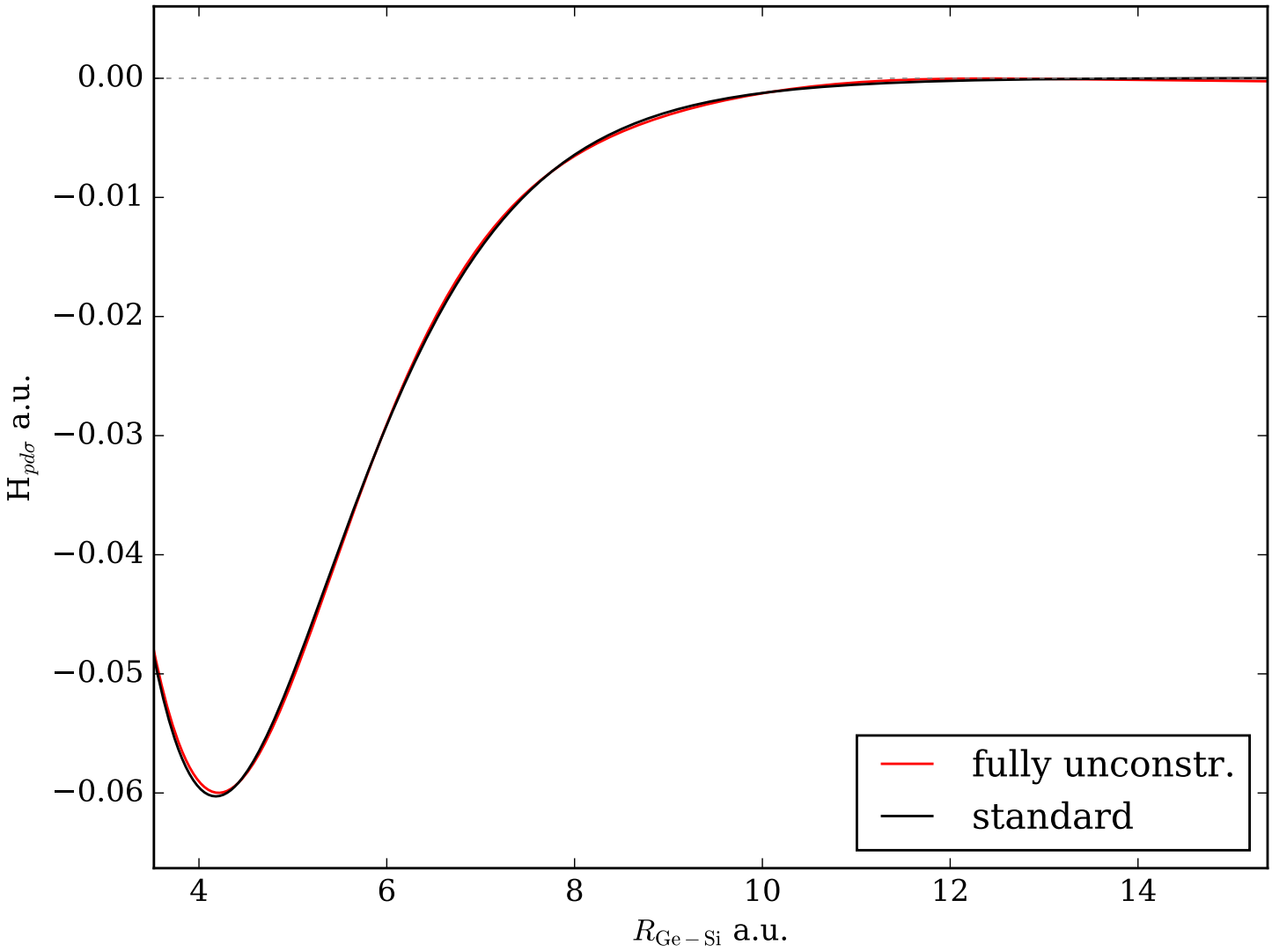
12 Ge-Si

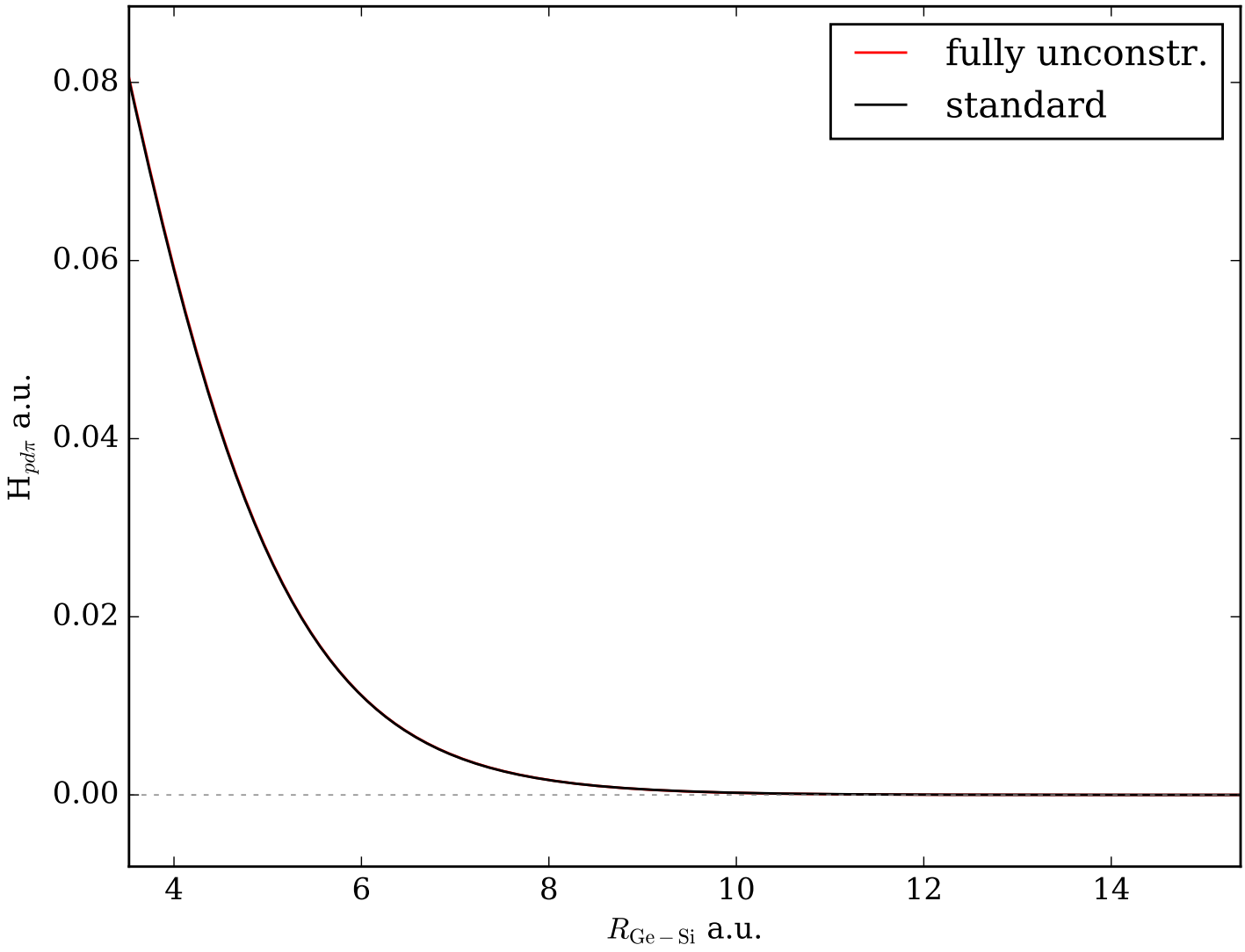
12.1 Electronic

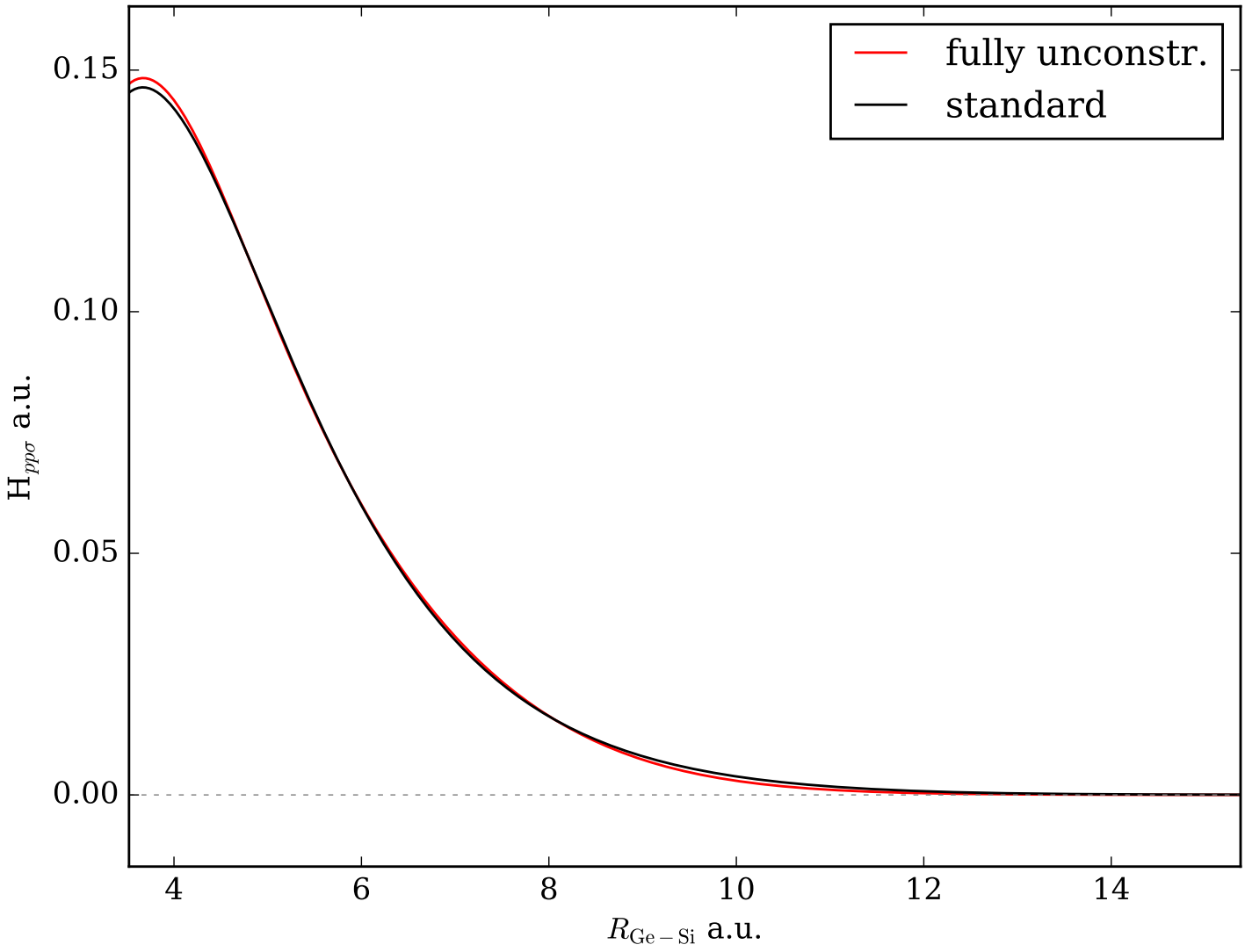


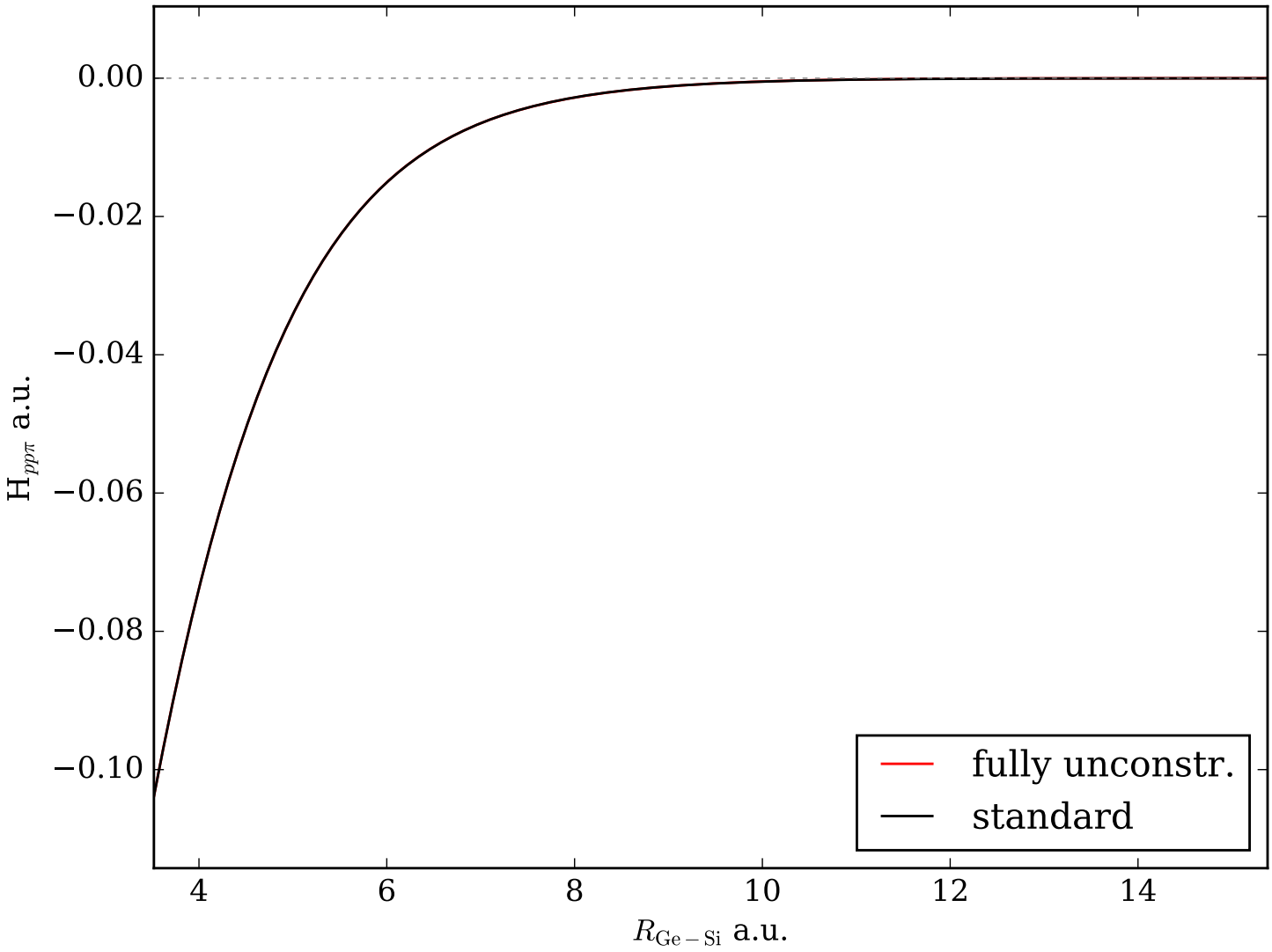

fully unconstr.
standard
0.05
0.04
0.03
0.02
0.01
0.00
$H_{dd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.


0.000
−0.005
−0.010
−0.015
−0.020
−0.025
$H_{dd\delta}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.
fully unconstr.
standard


0.00
−0.01
−0.02
−0.03
−0.04
−0.05
−0.06
$H_{pd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.08
0.06
0.04
0.02
0.00
$H_{pd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.


fully unconstr.
standard
0.15
0.10
0.05
0.00
$H_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.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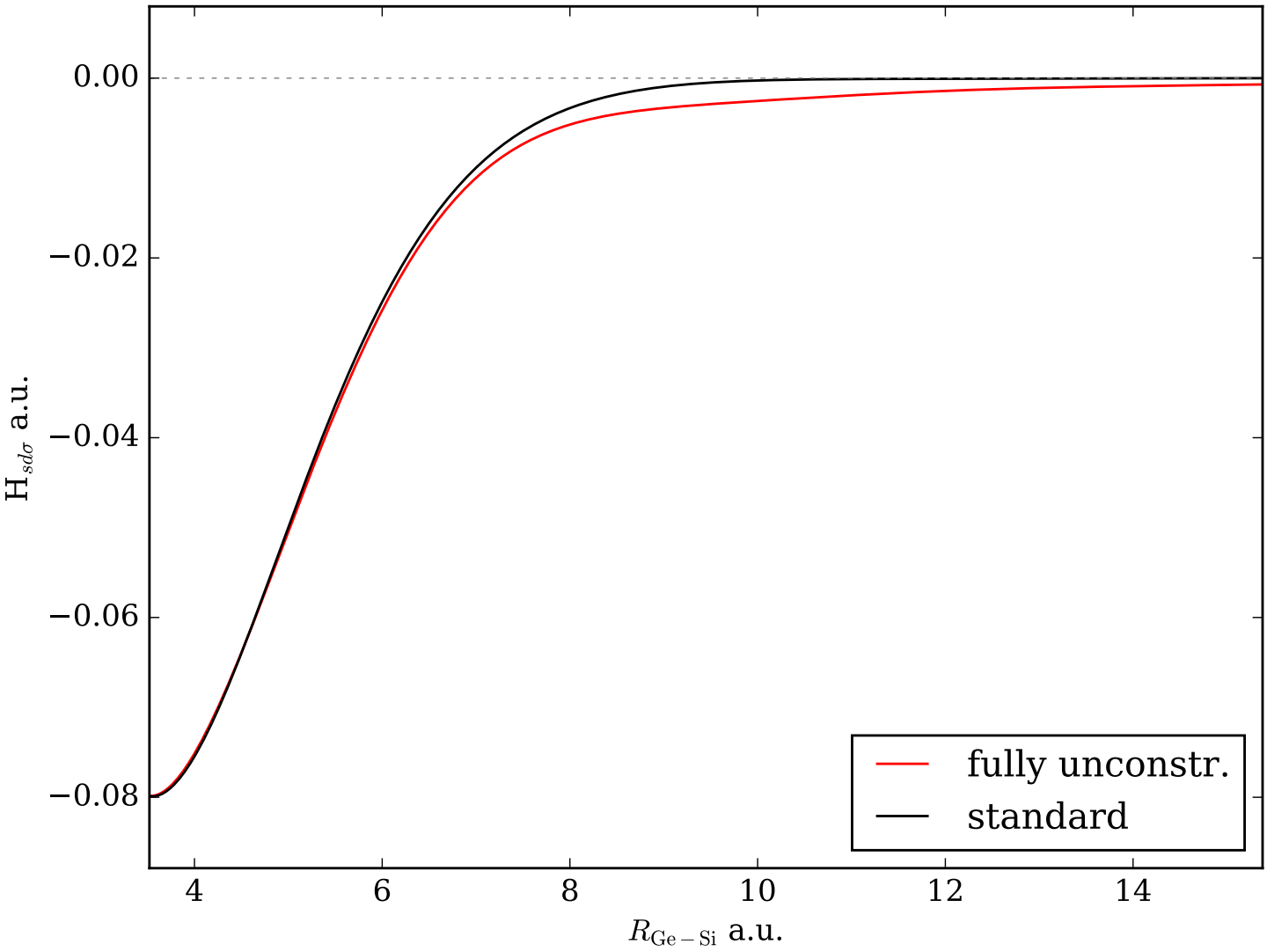
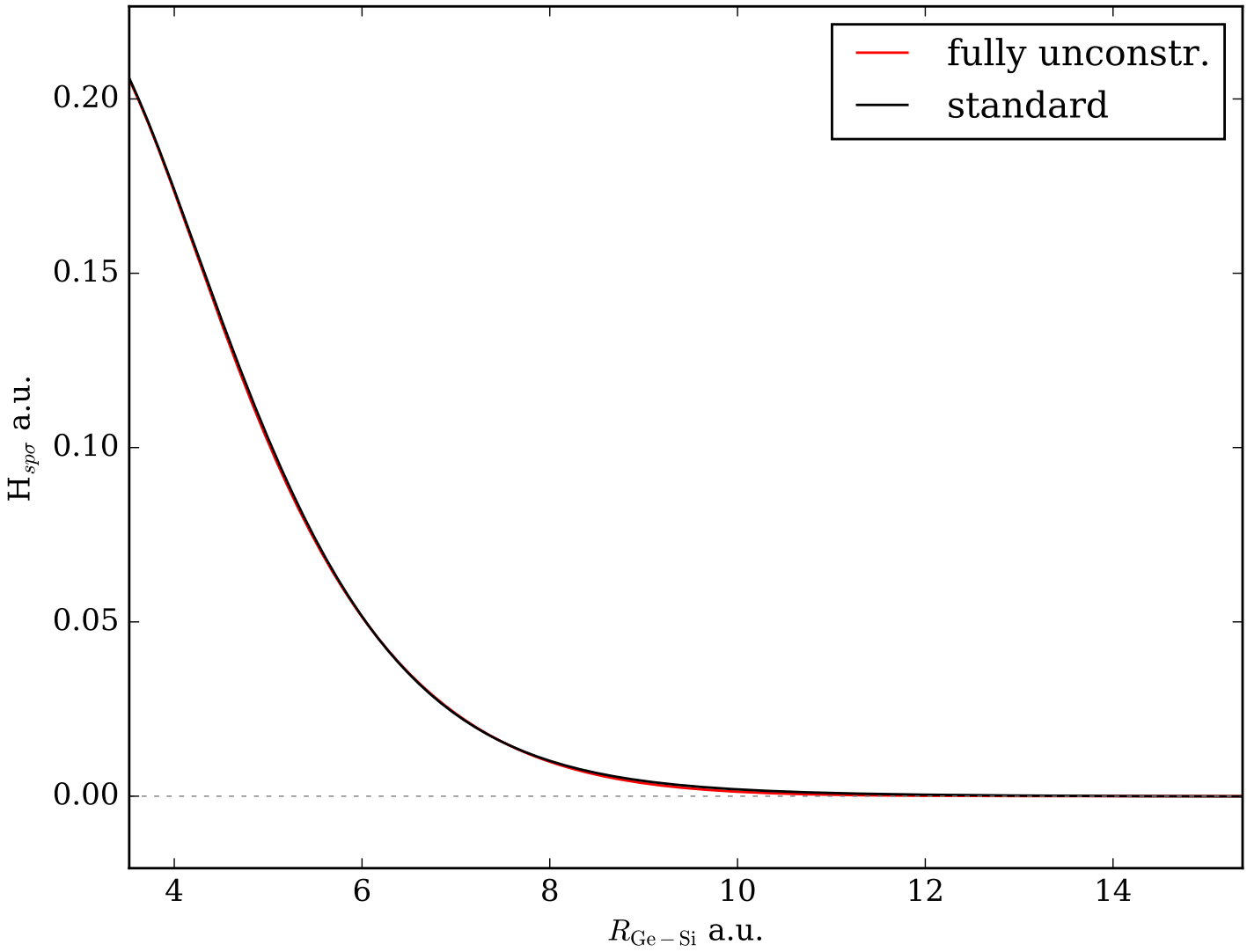
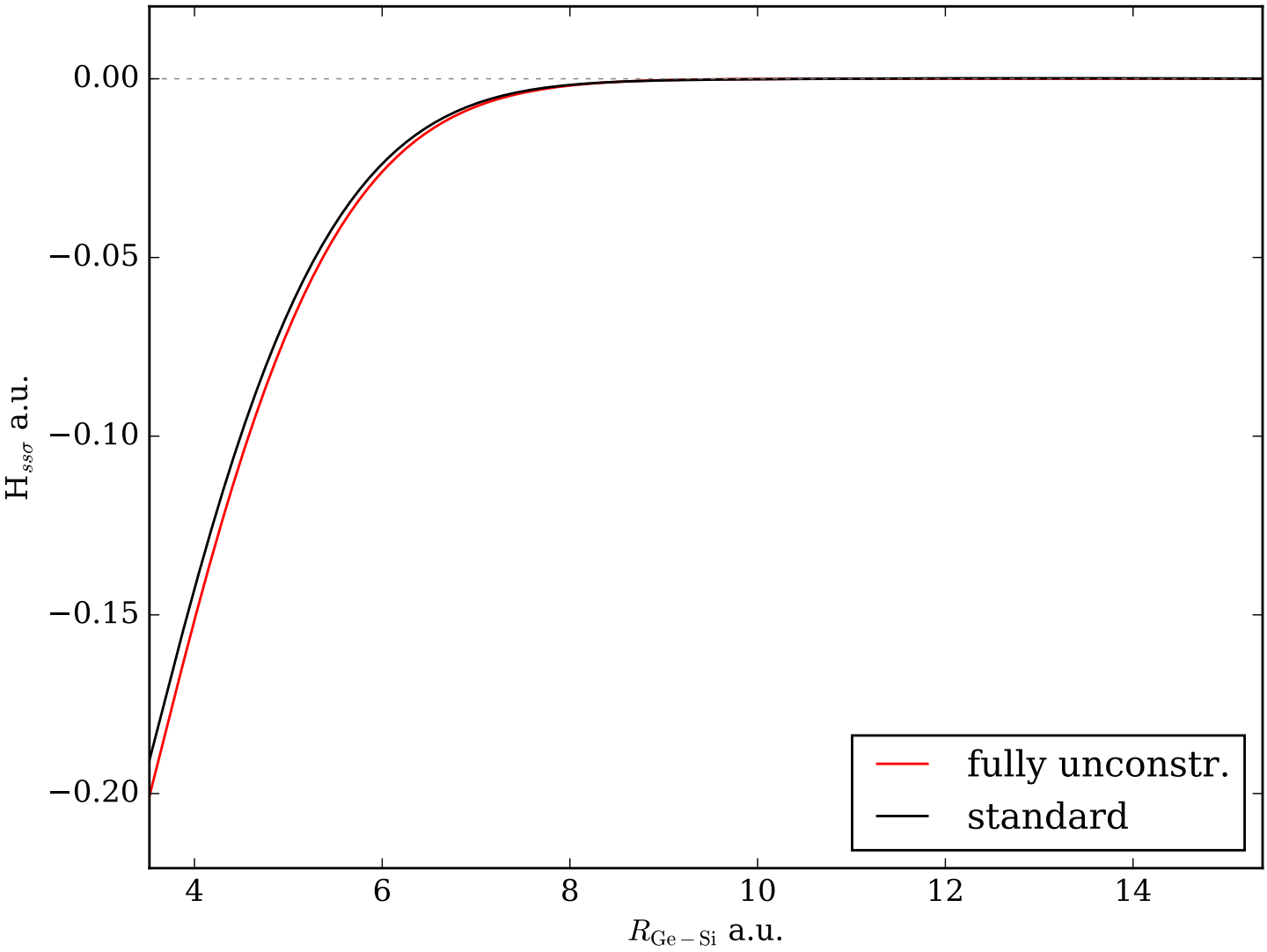
−0.02
−0.04
−0.06
−0.08
−0.10
$H_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.
fully unconstr.
standard


0.00
−0.02
−0.04
−0.06
−0.08
$H_{sd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.20
0.15
0.10
0.05
0.00
$H_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.


0.00
−0.05
−0.10
−0.15
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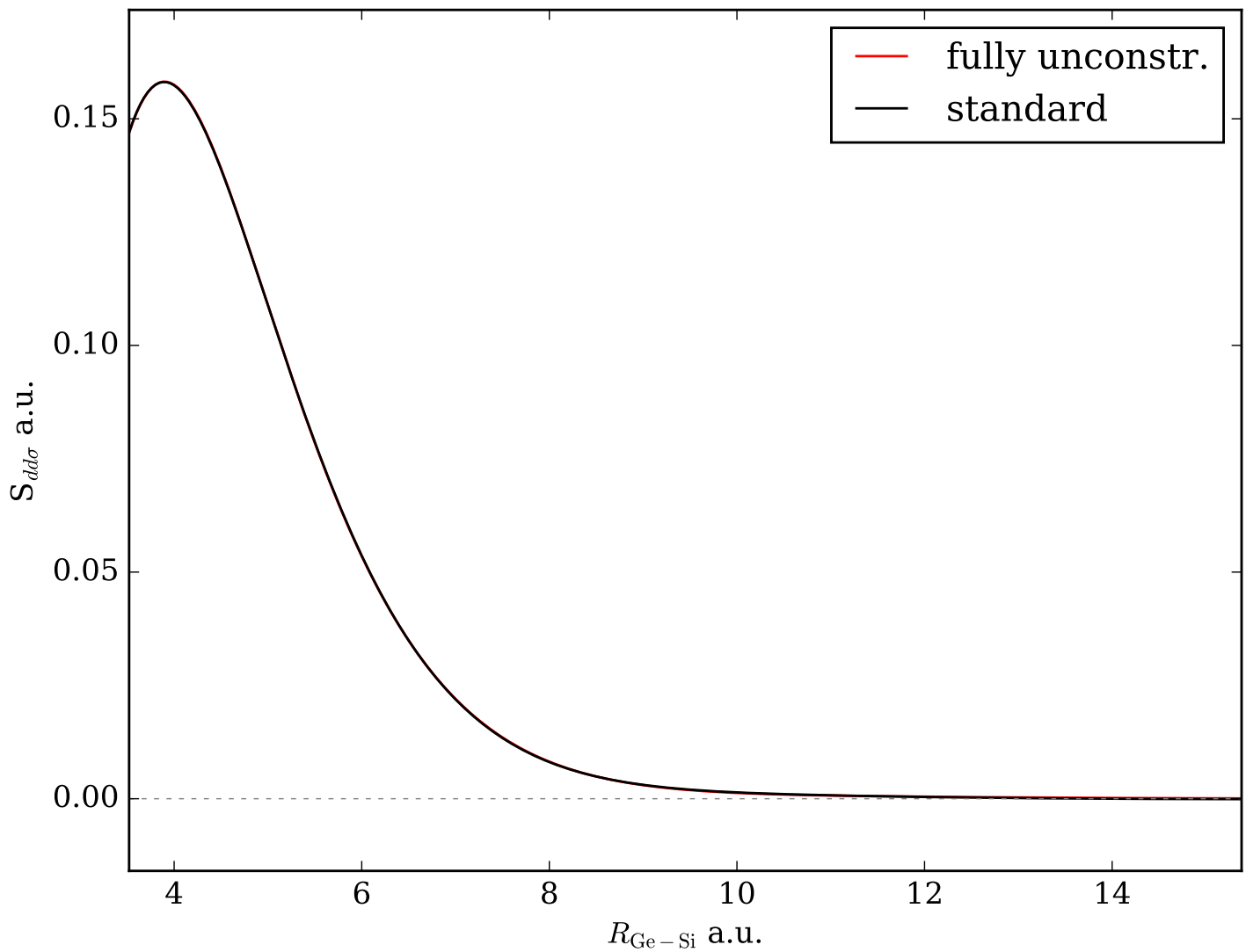
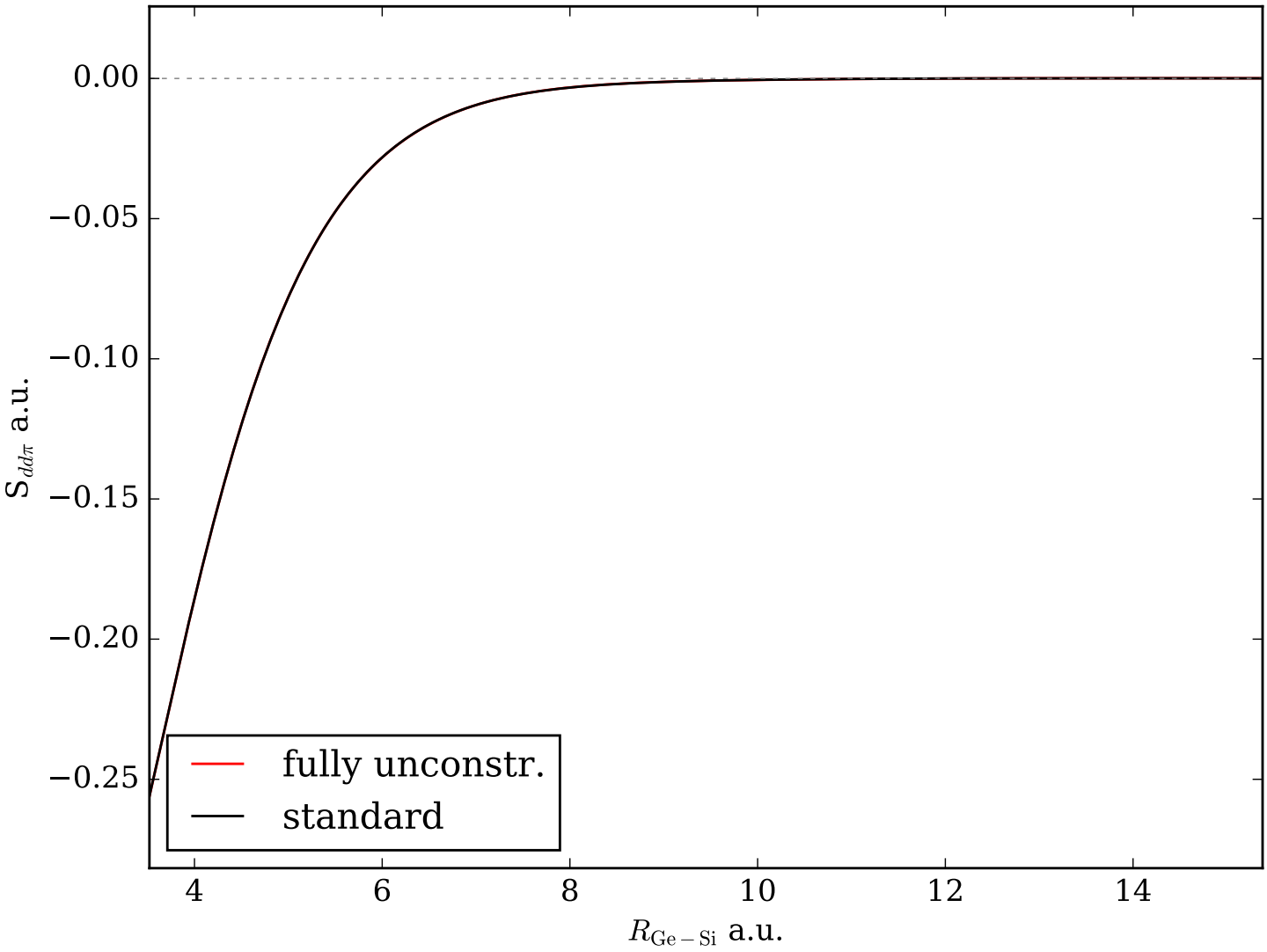
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.15
0.10
0.05
0.00
$S_{dd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.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−0.10
−0.15
−0.20
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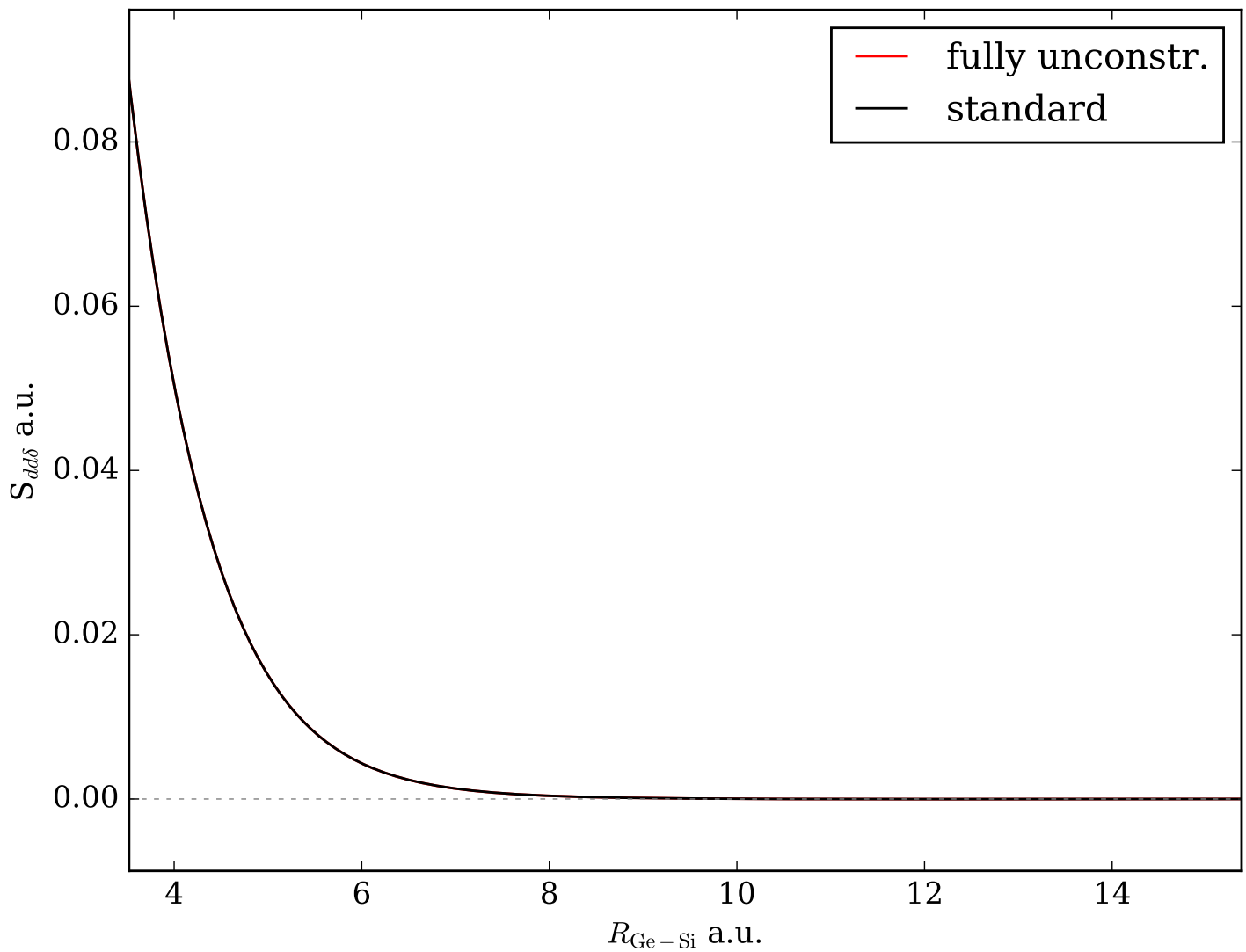
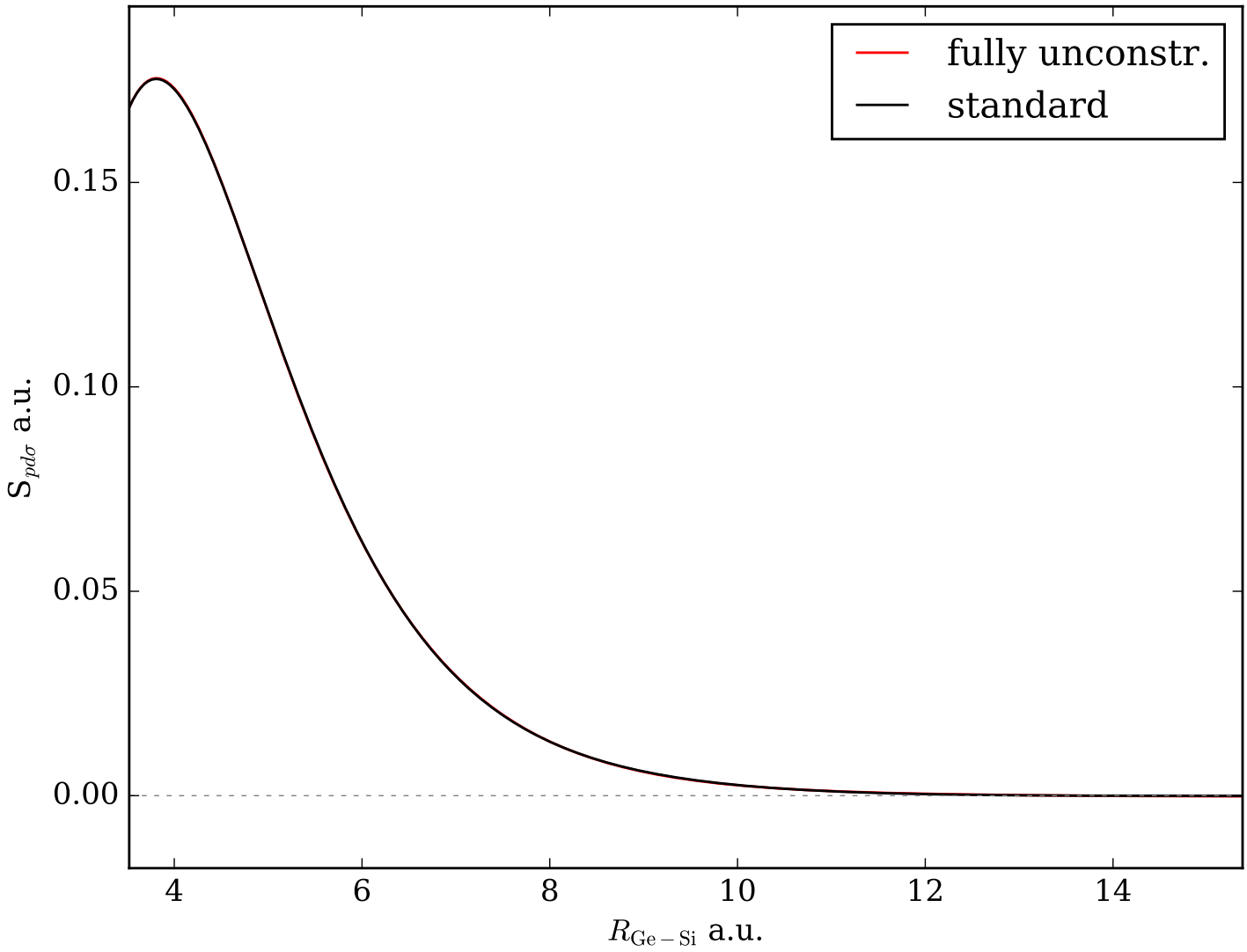
$S_{dd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.08
0.06
0.04
0.02
0.00
$S_{dd\delta}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.


fully unconstr.
standard
0.15
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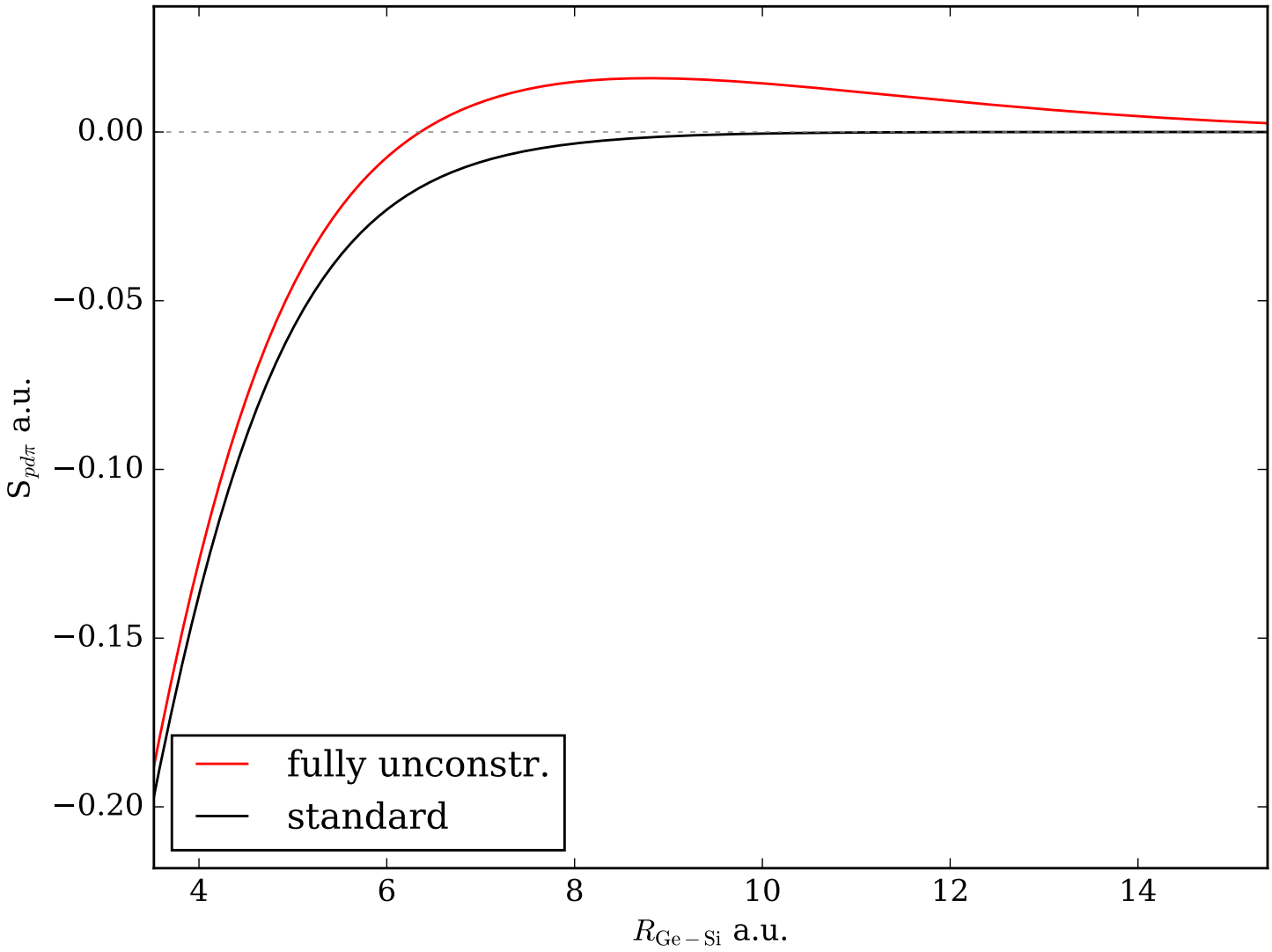
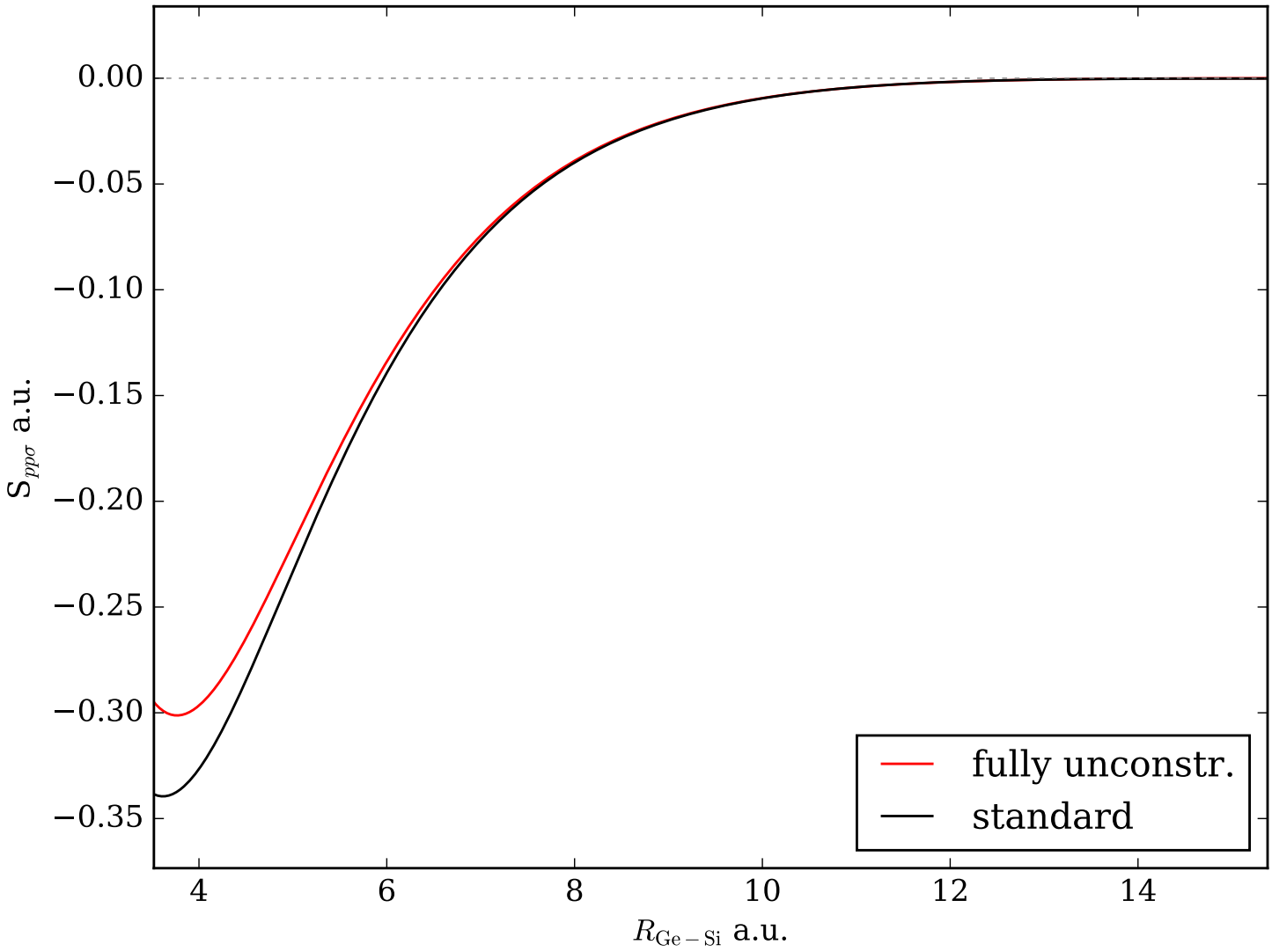
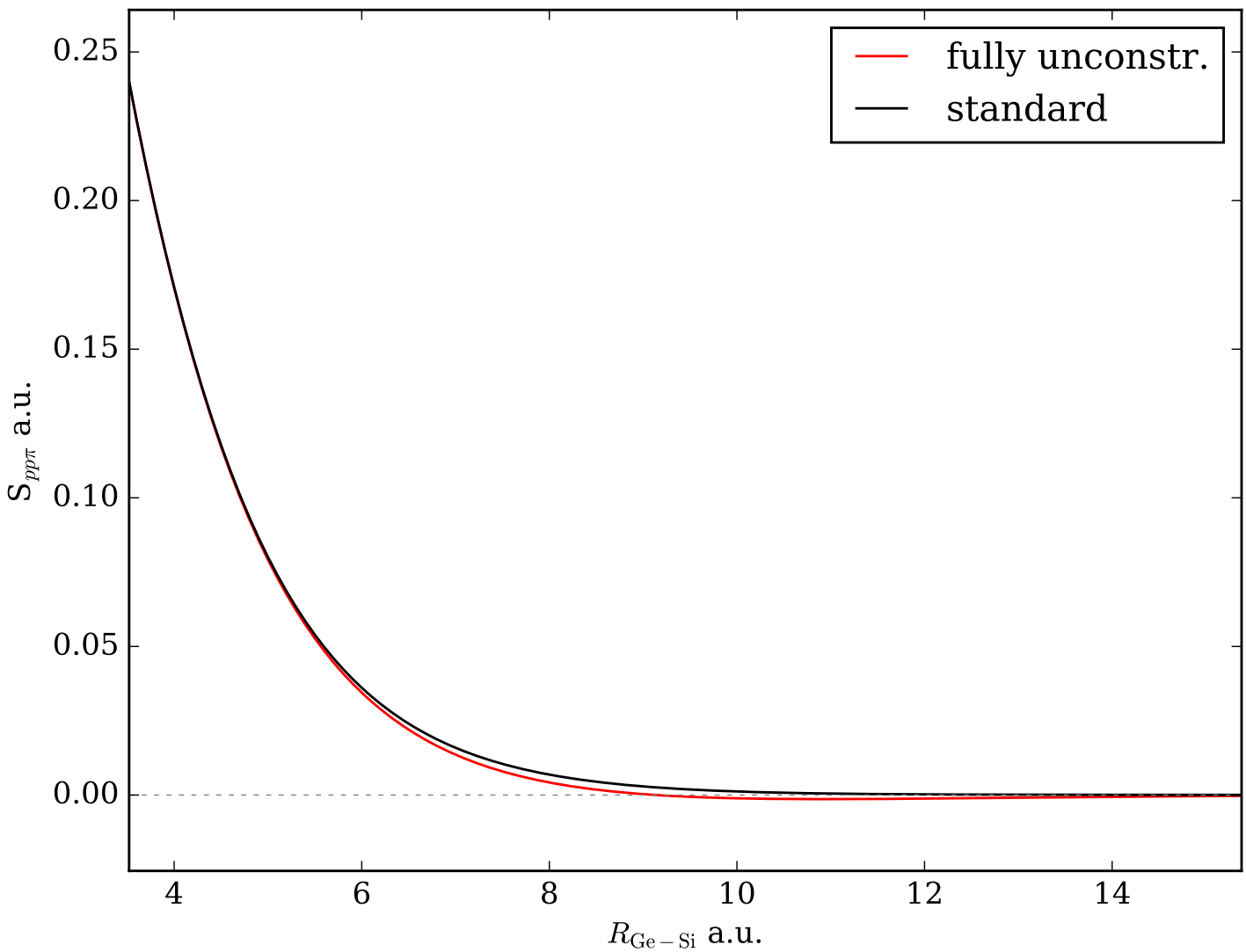
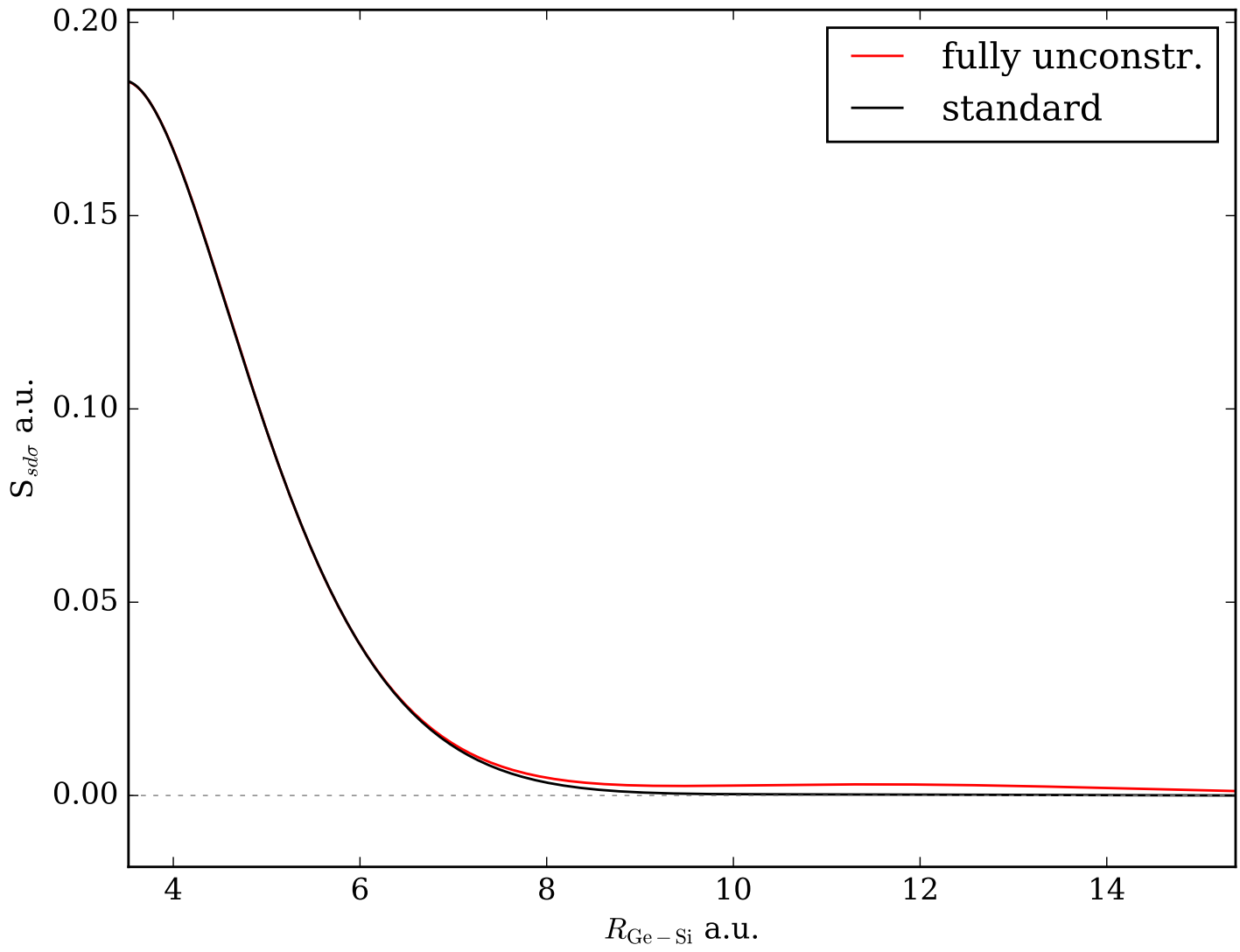
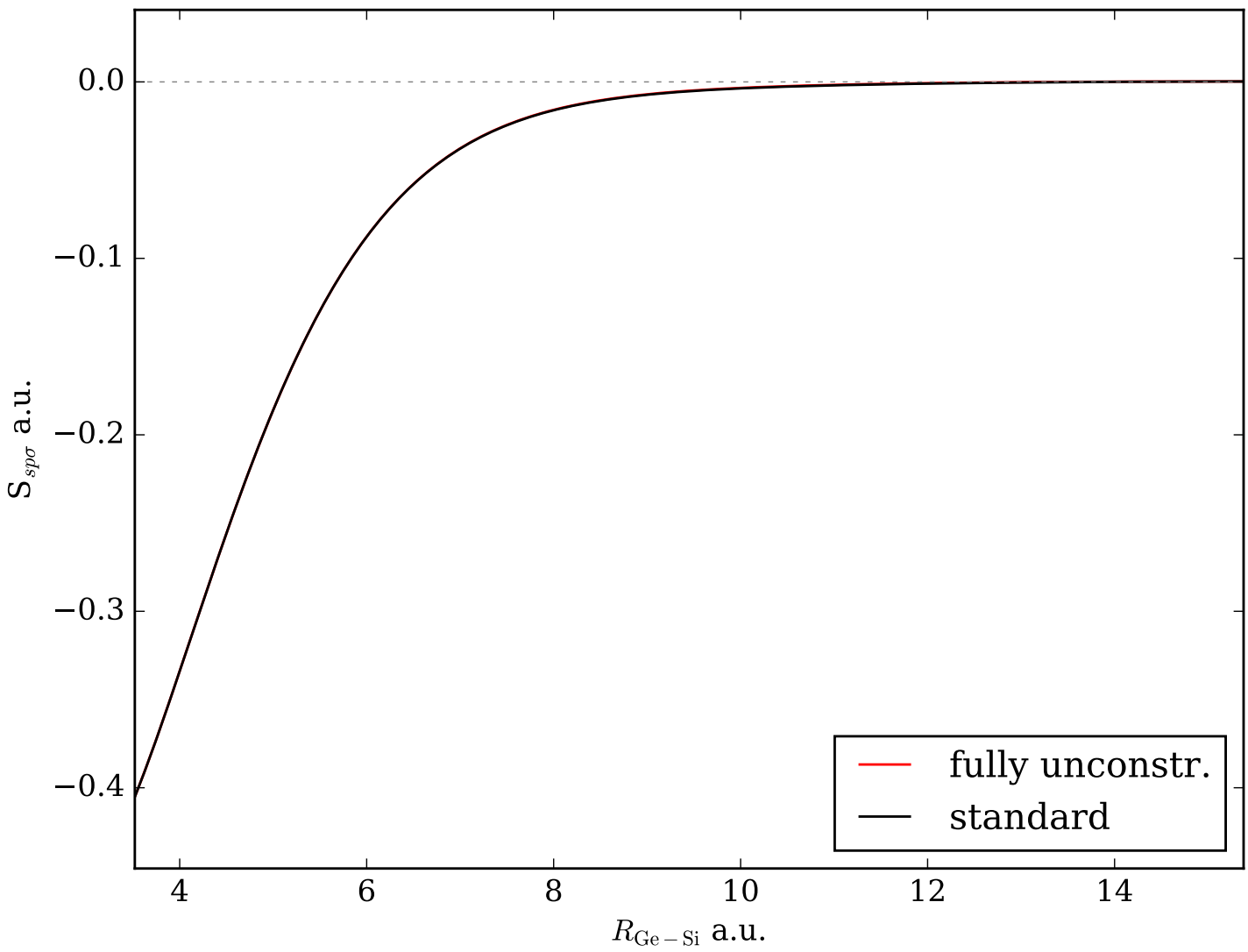
0.05
0.00
$S_{pd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.

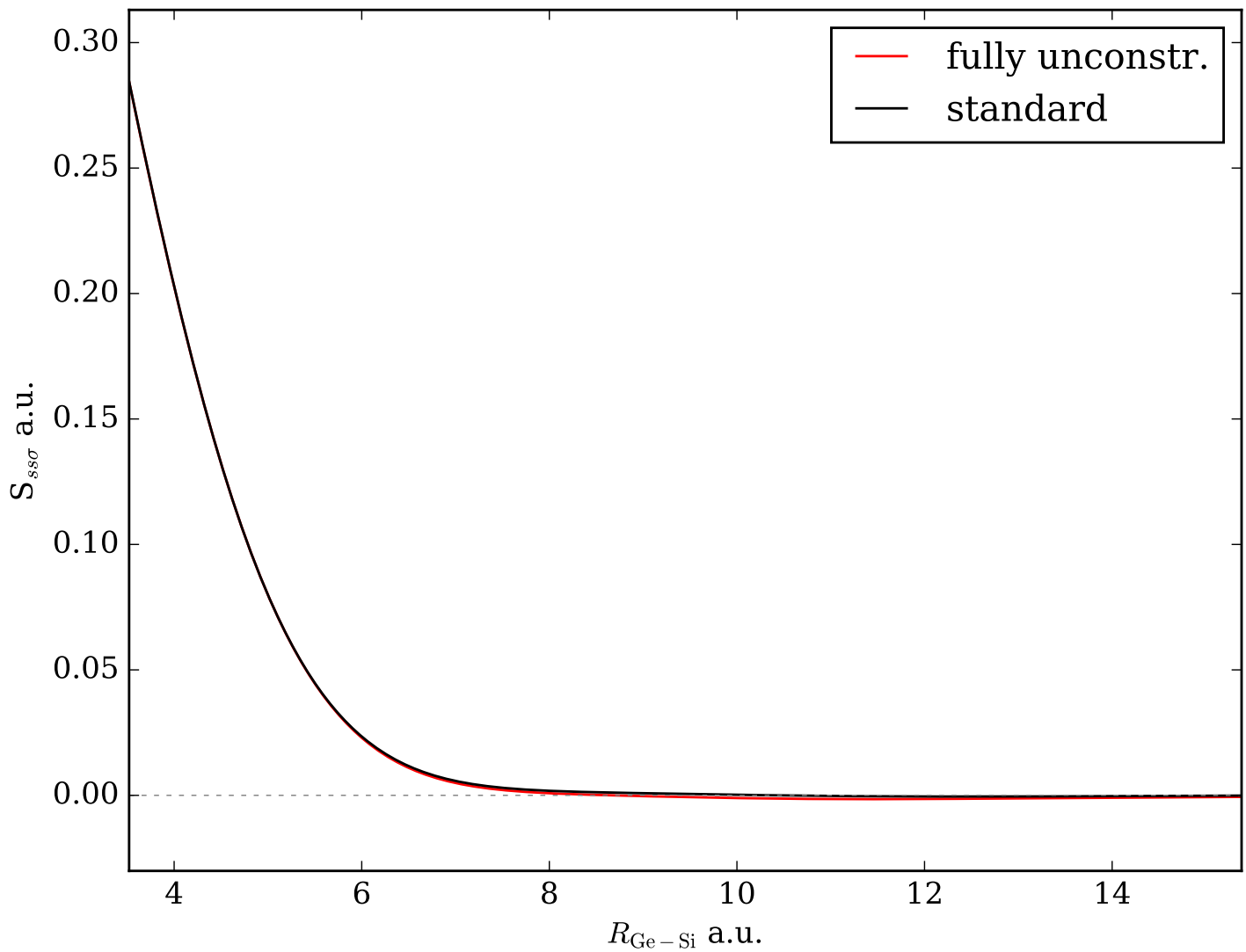

0.00
−0.05
−0.10
−0.15
−0.20
$S_{pd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.
fully unconstr.
standard


0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
−0.35
$S_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.25
0.20
0.15
0.10
0.05
0.00
$S_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.

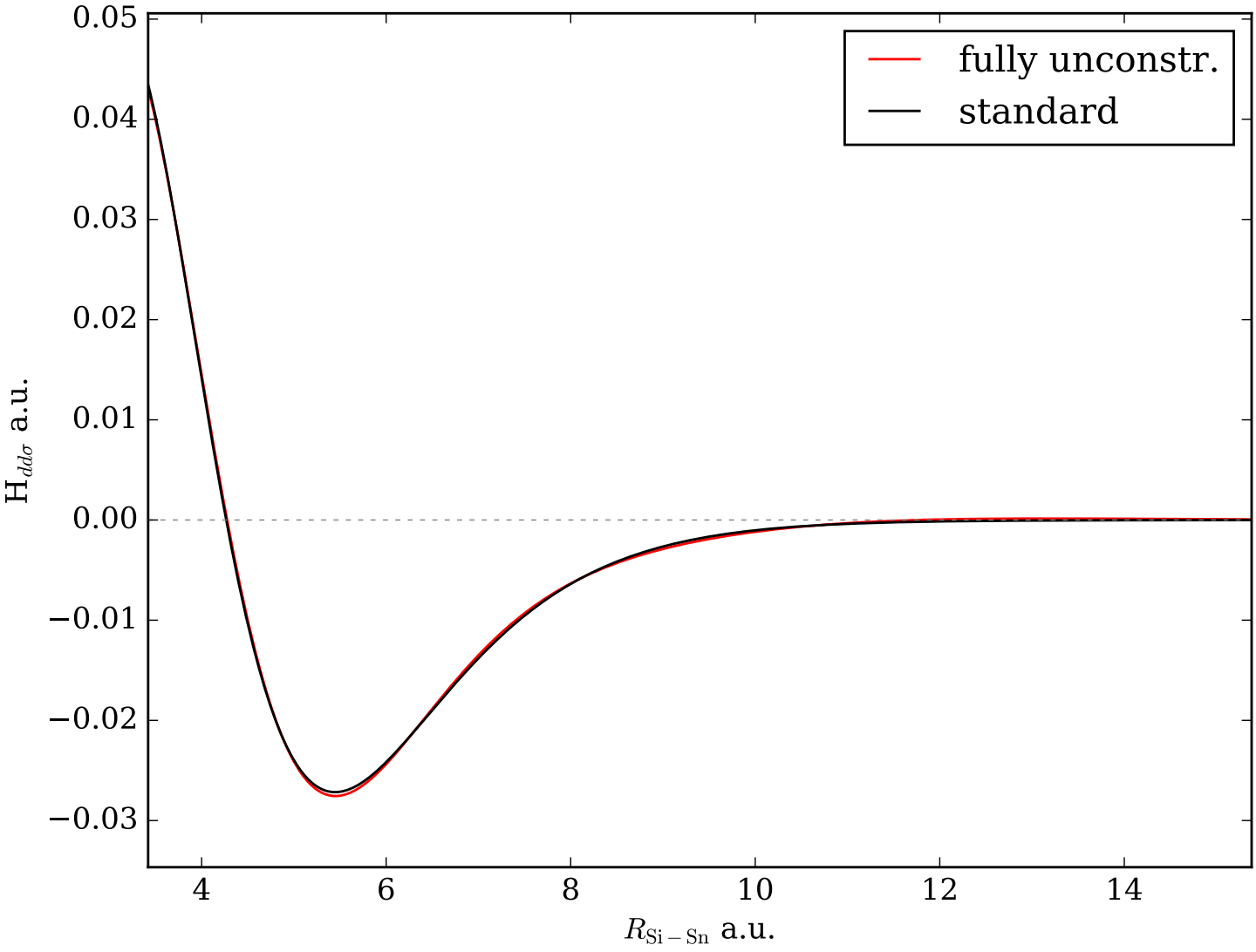

fully unconstr.
standard
0.20
0.15
0.10
0.05
0.00
4
6
8
10
12
14
$S_{sd\sigma}$ a.u.
$R_{\mathrm{Ge-Si}}$ a.u.

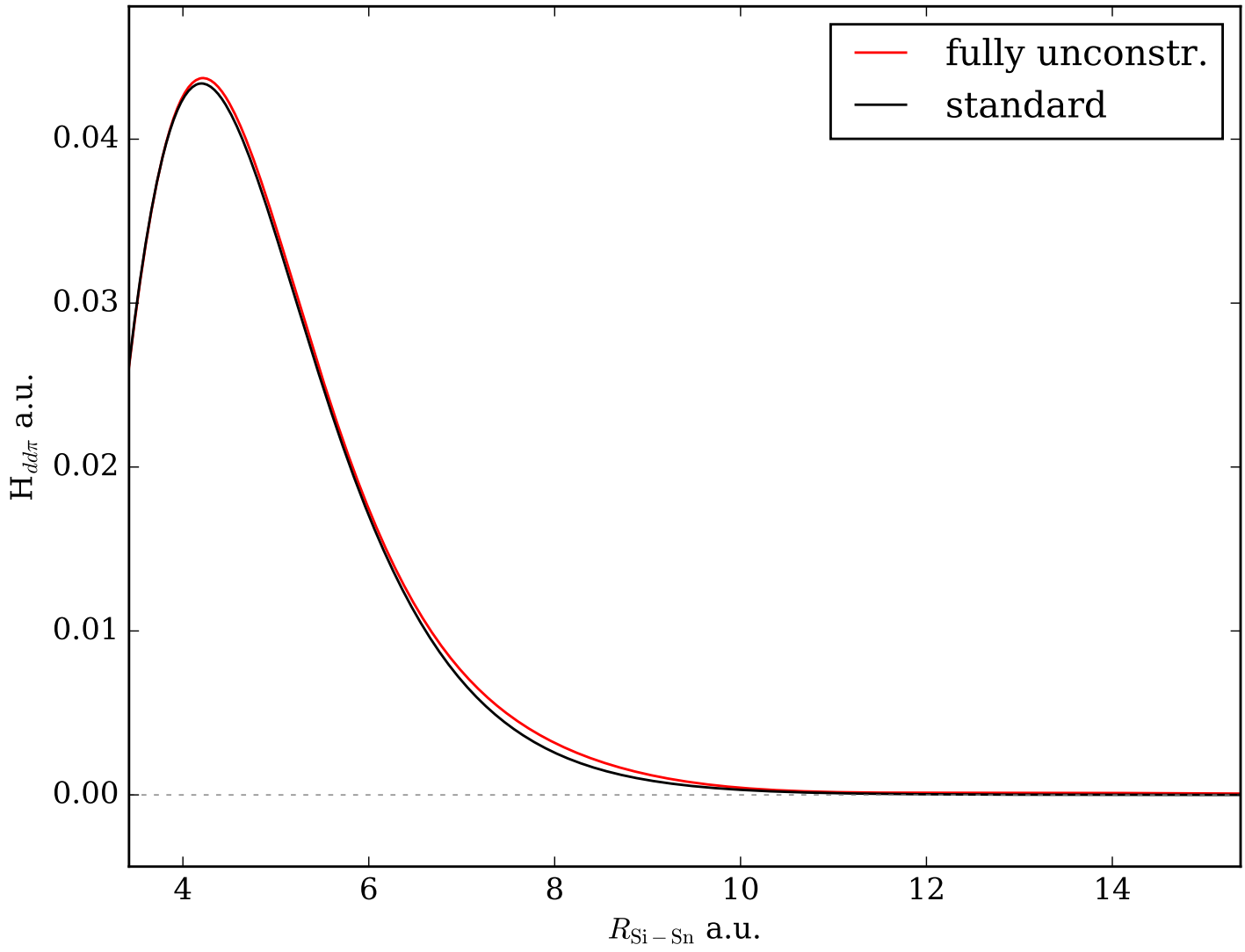

0.0
−0.1
−0.2
−0.3
−0.4
$S_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.
fully unconstr.
standard

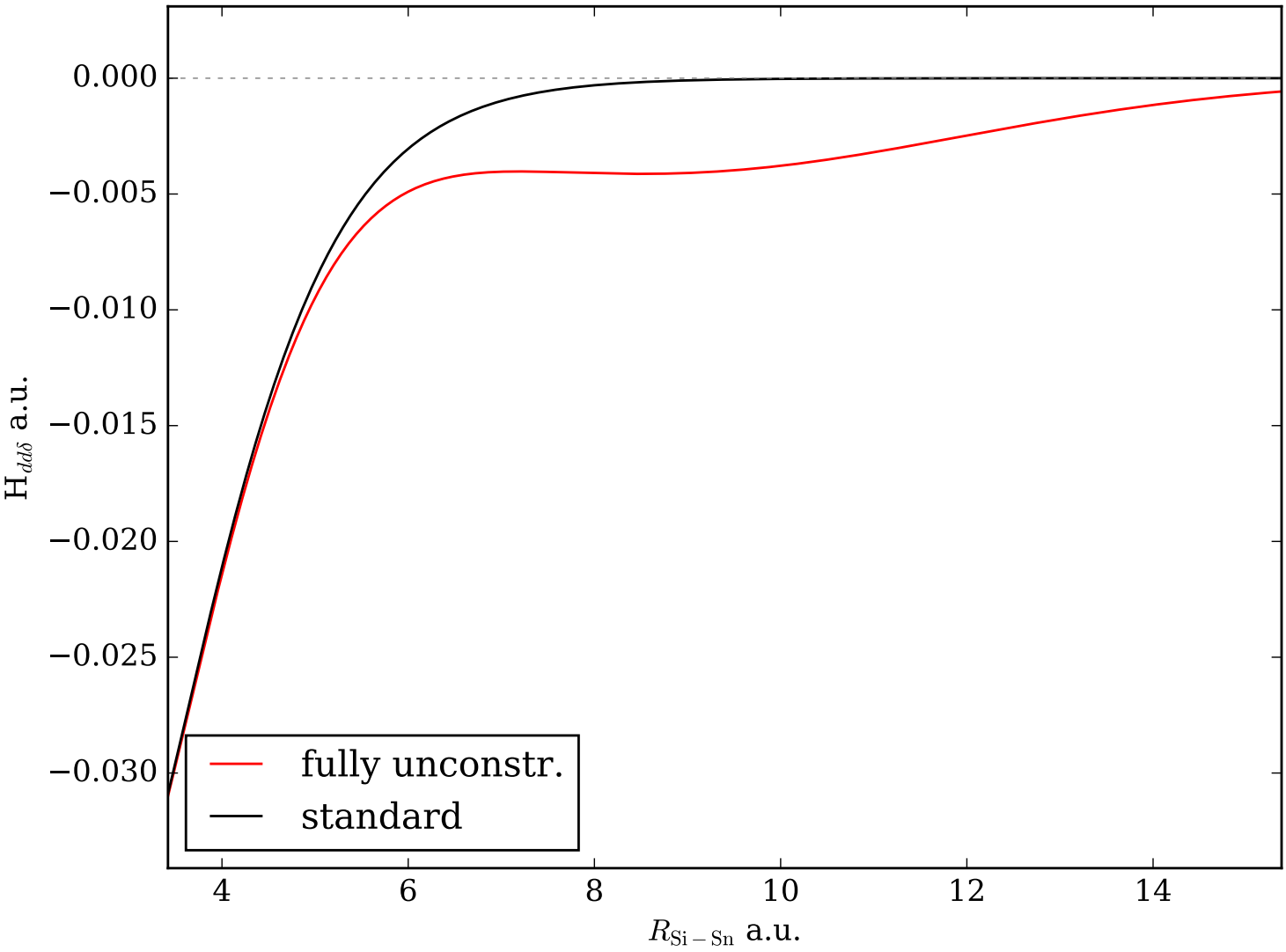

fully unconstr.
standard
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$S_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Si}}$ a.u.

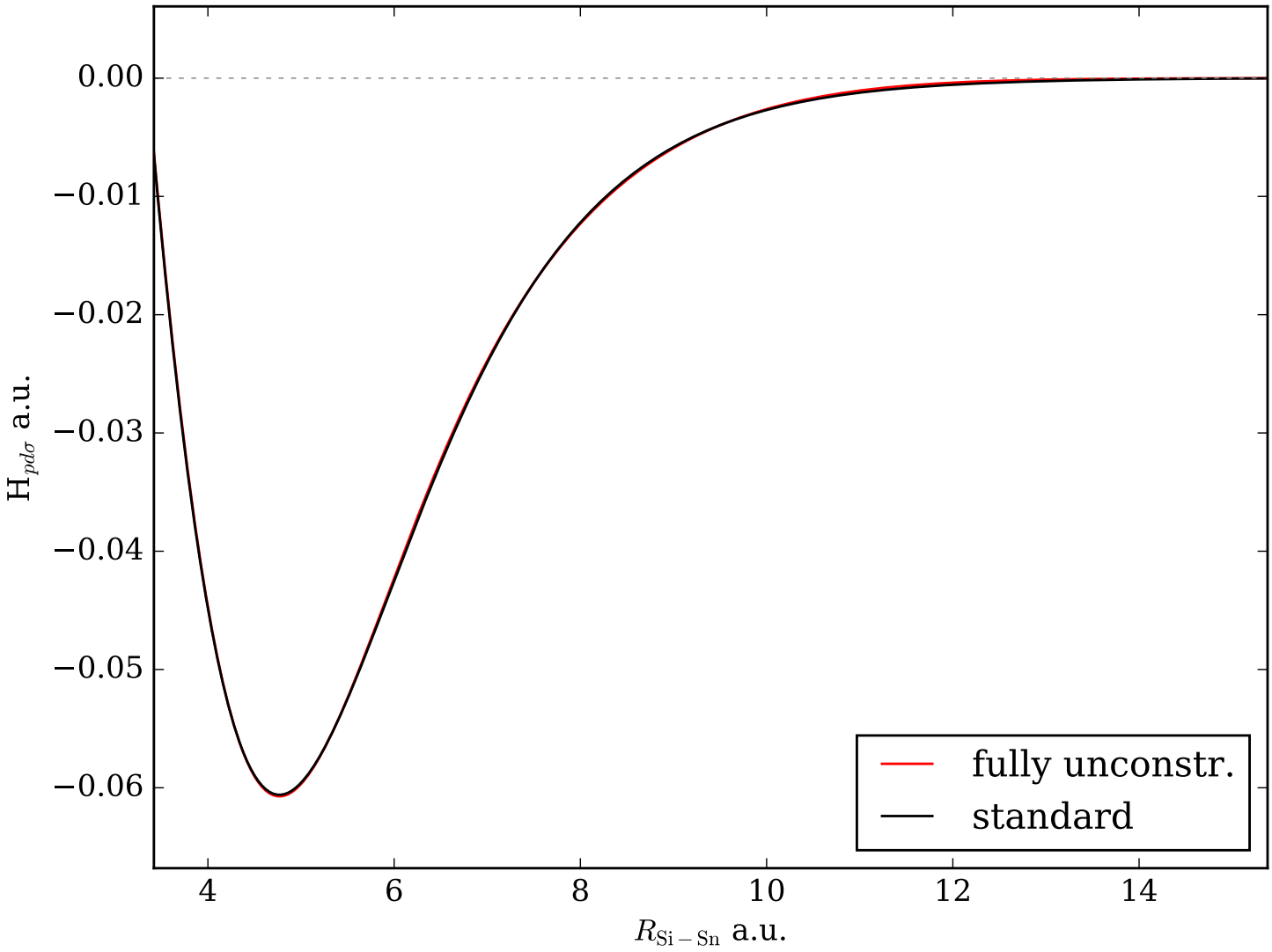
13 Si-Sn

13.1 Electronic




fully unconstr.
standard
0.04
0.03
0.02
0.01
0.00
$H_{dd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.


0.000
−0.005
−0.010
−0.015
−0.020
−0.025
−0.030
$H_{dd\delta}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.
fully unconstr.
standard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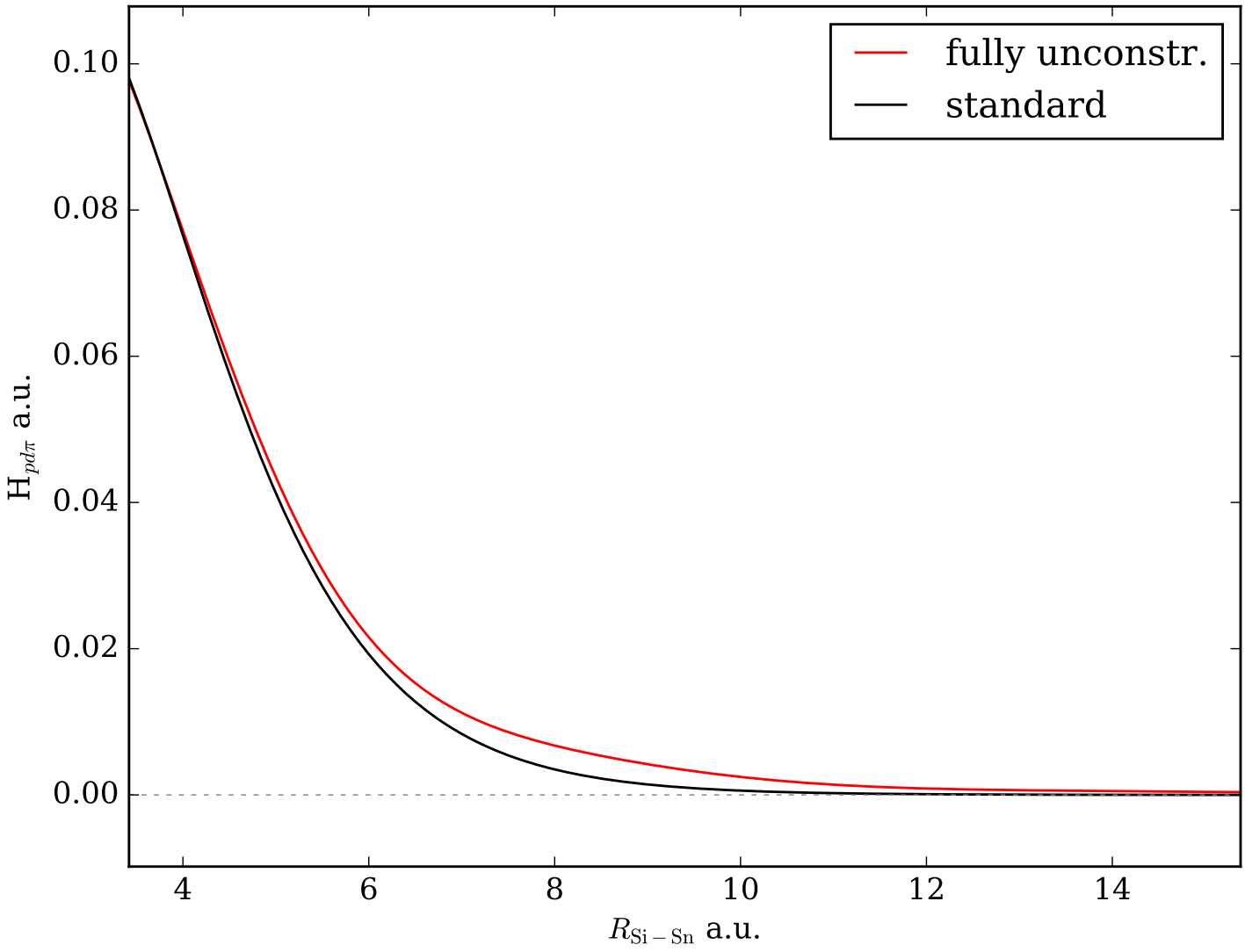
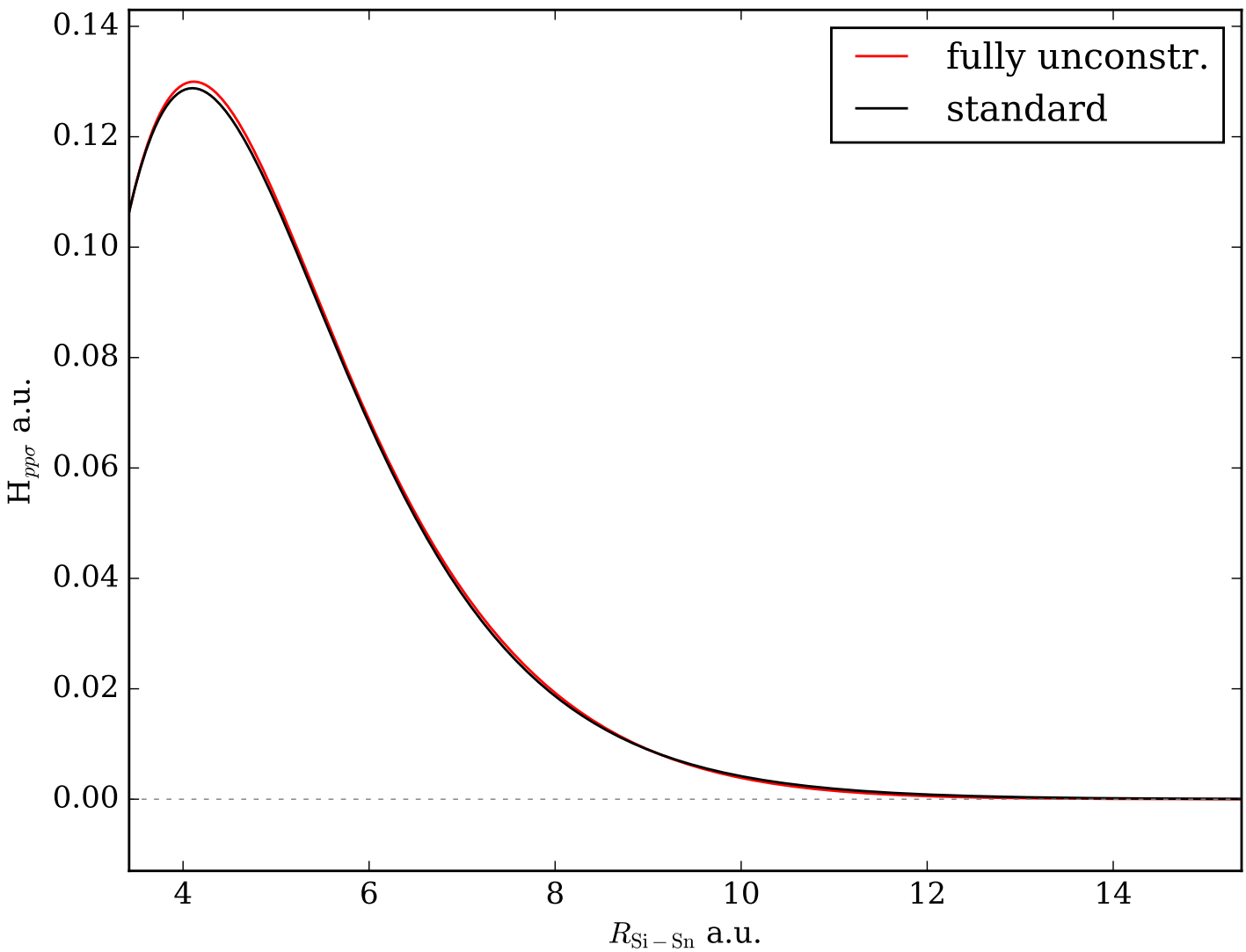
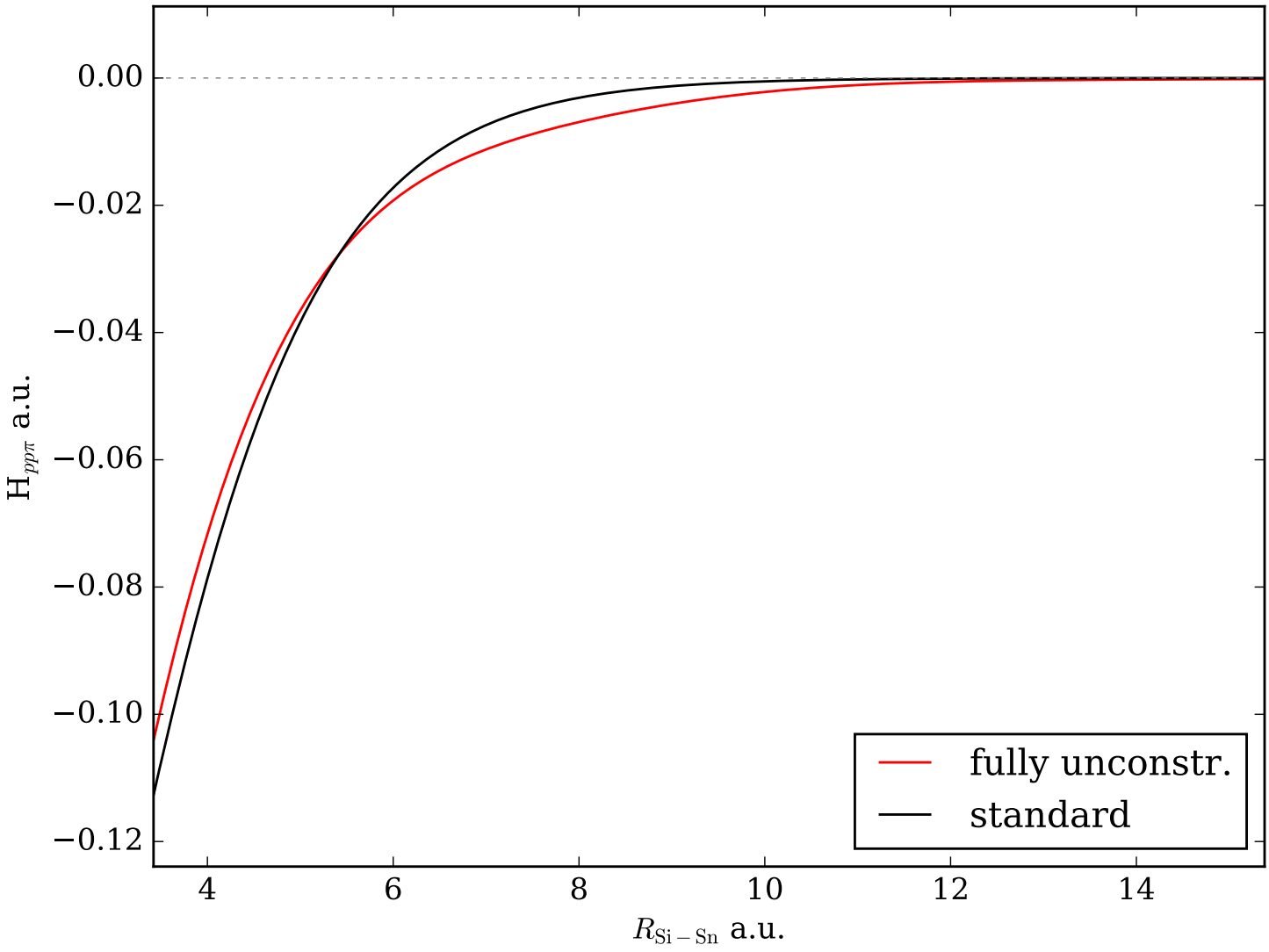
−0.01
−0.02
−0.03
−0.04
−0.05
−0.06
$H_{pd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.10
0.08
0.06
0.04
0.02
0.00
$H_{pd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.


fully unconstr.
standard
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
$H_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.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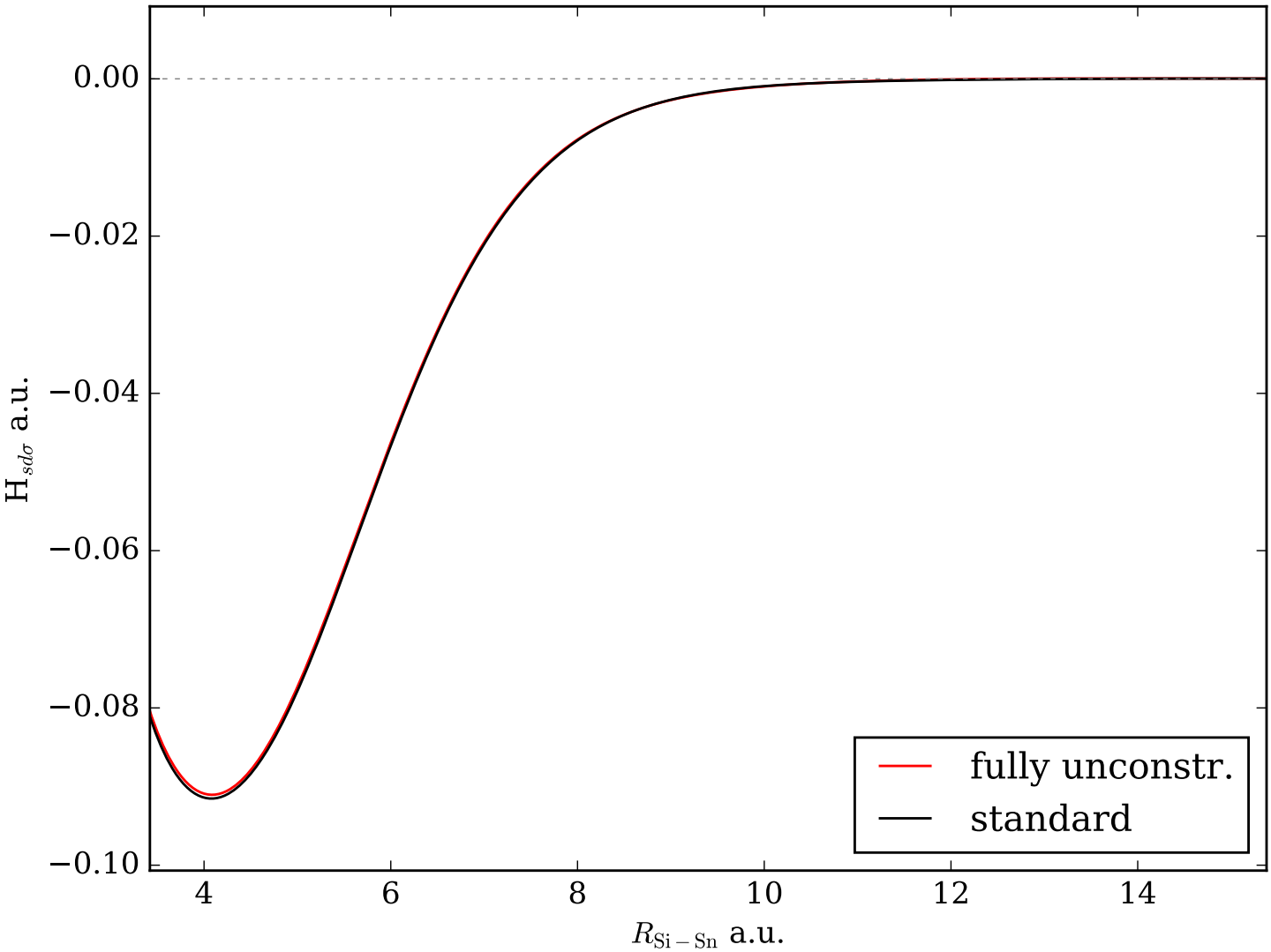
−0.02
−0.04
−0.06
−0.08
−0.10
−0.12
$H_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.
fully unconstr.
standard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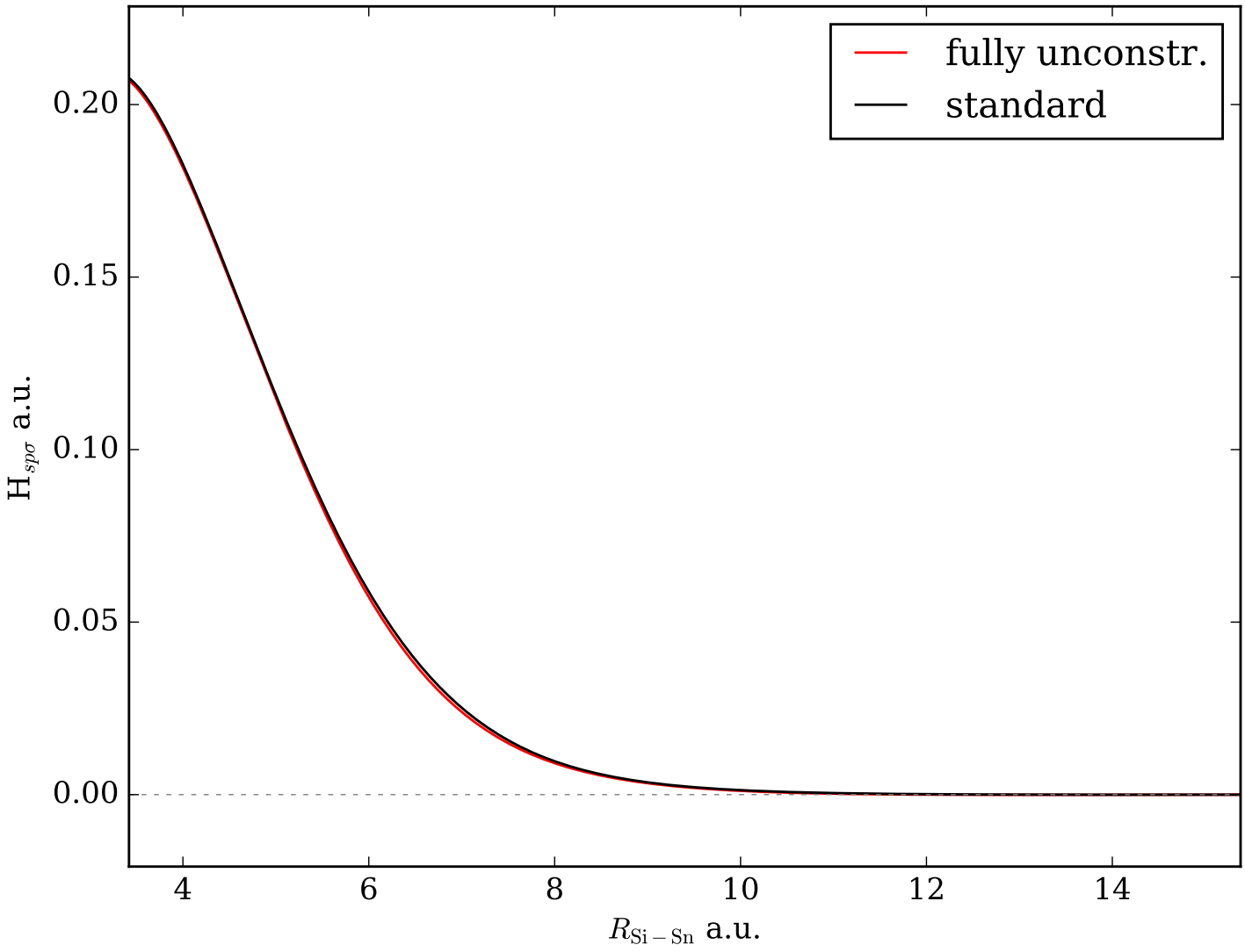
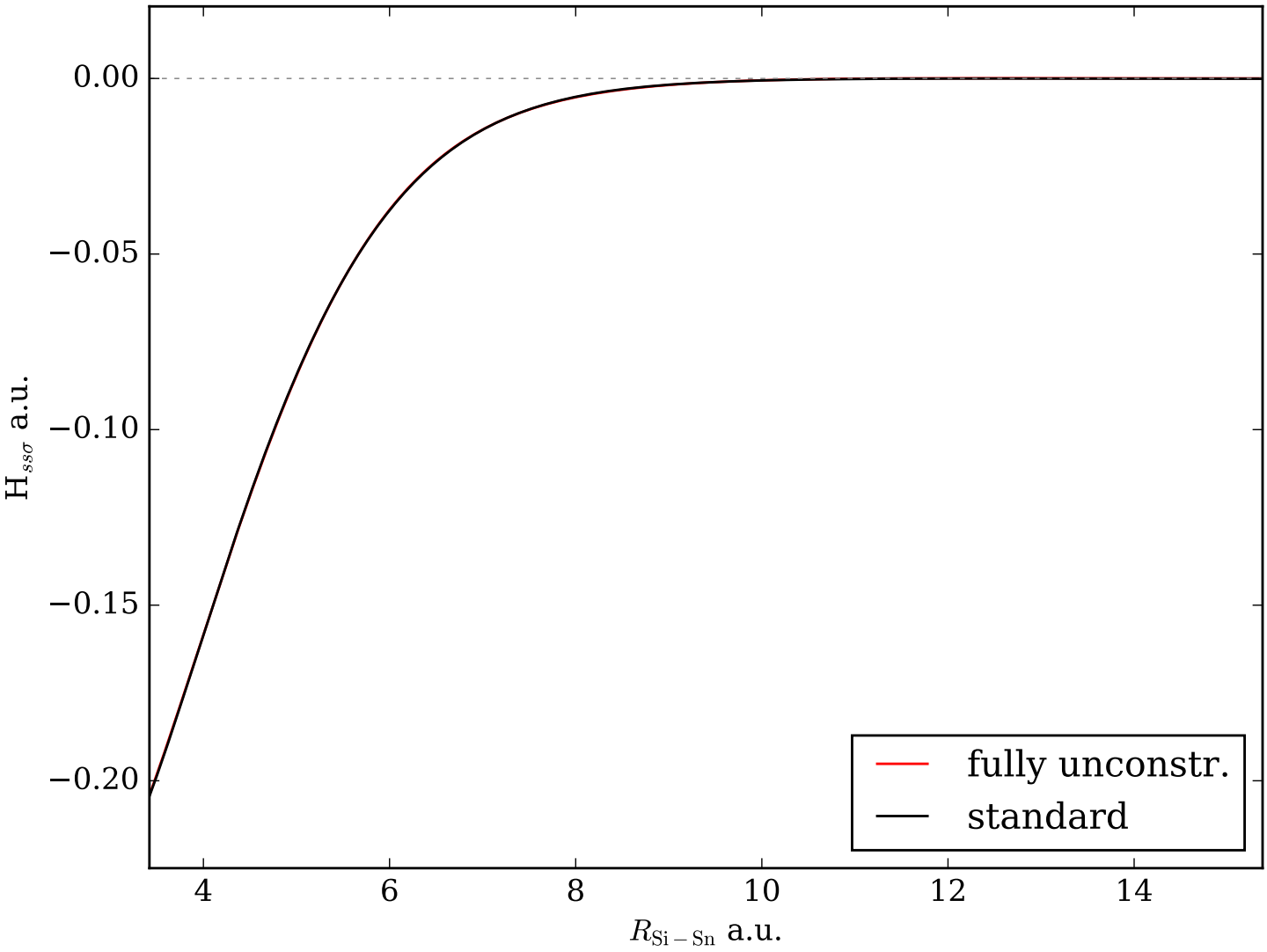
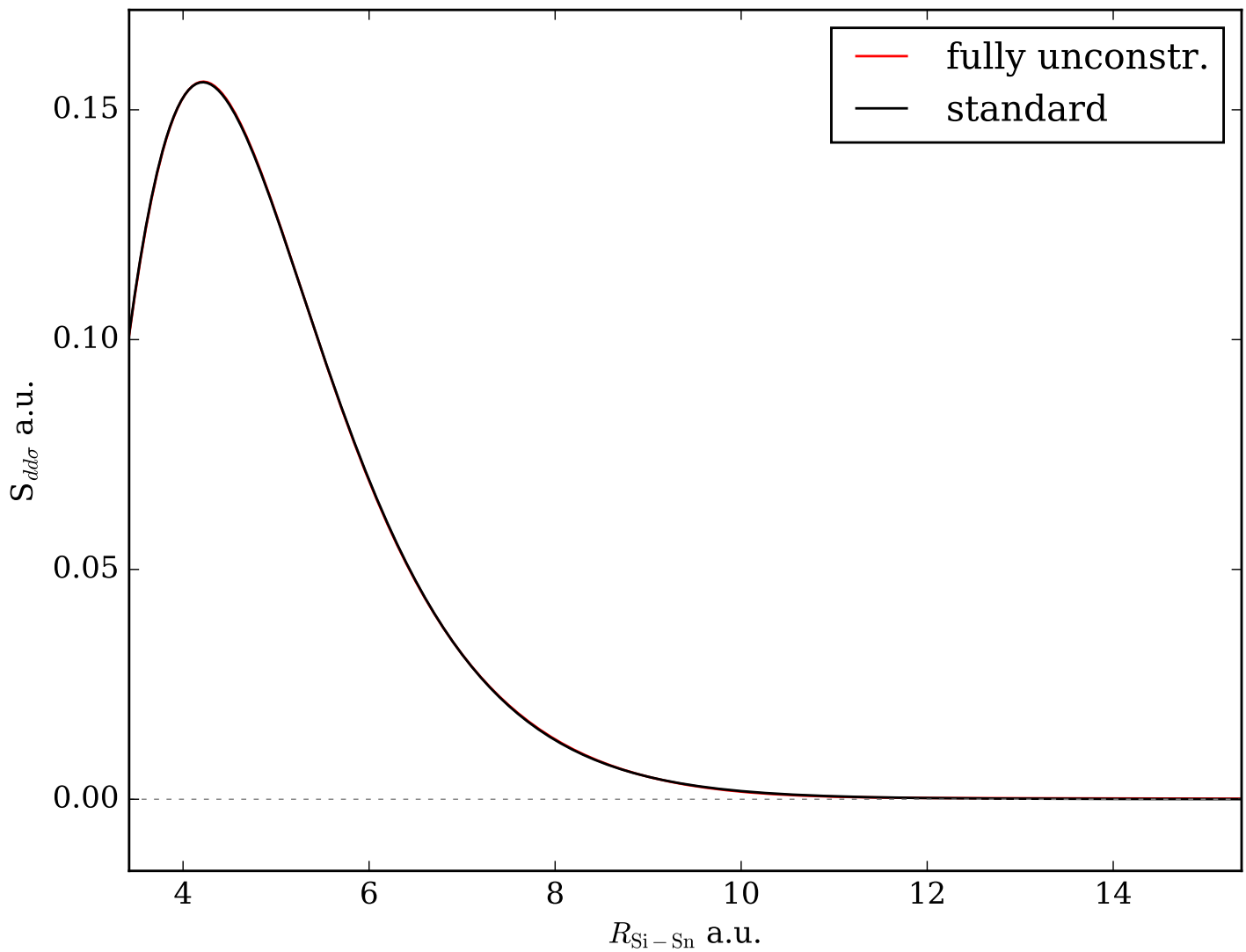
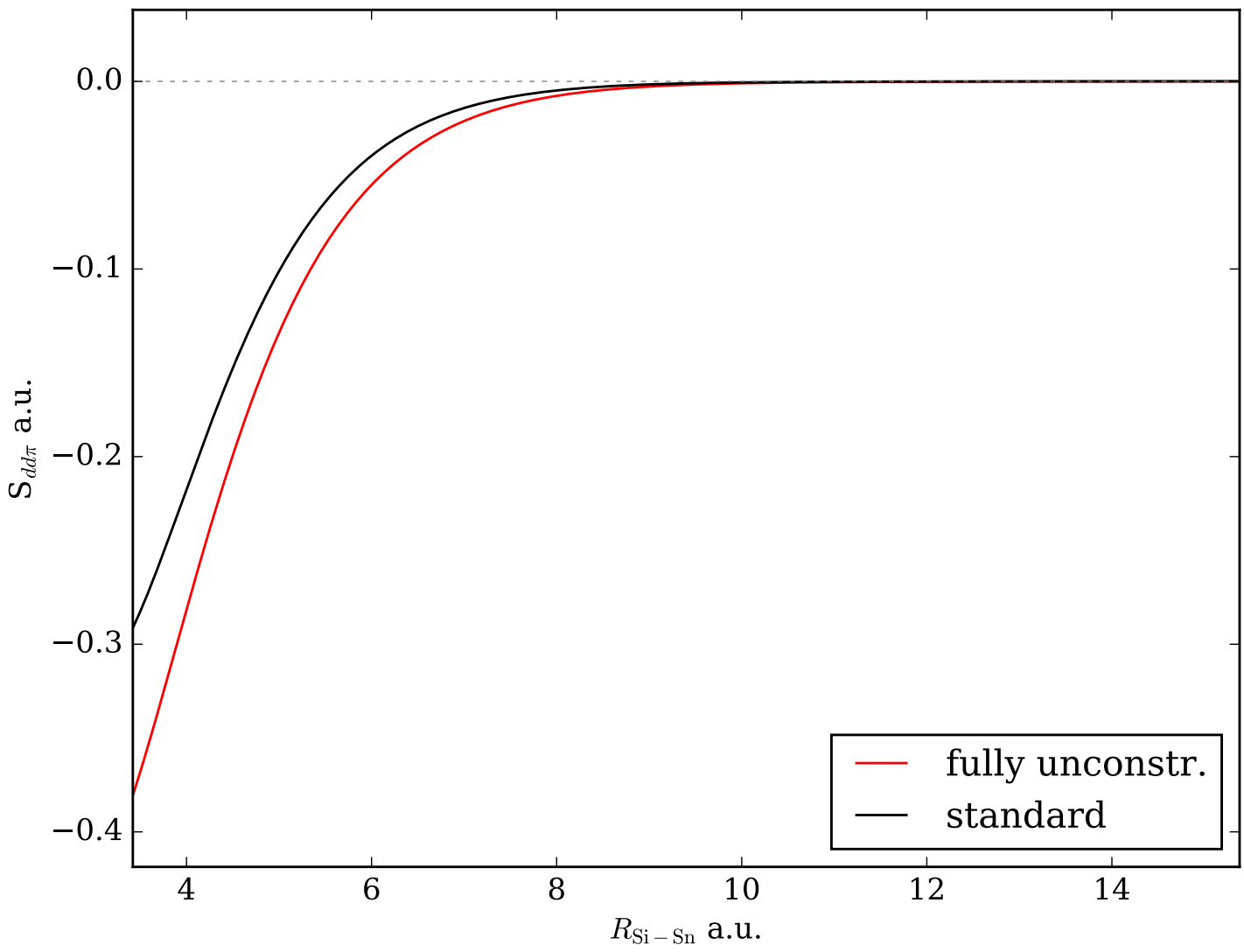
−0.02
−0.04
−0.06
−0.08
−0.10
$H_{sd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.20
0.15
0.10
0.05
0.00
$H_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.


0.00
−0.05
−0.10
−0.15
−0.20
$H_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.15
0.10
0.05
0.00
$S_{dd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.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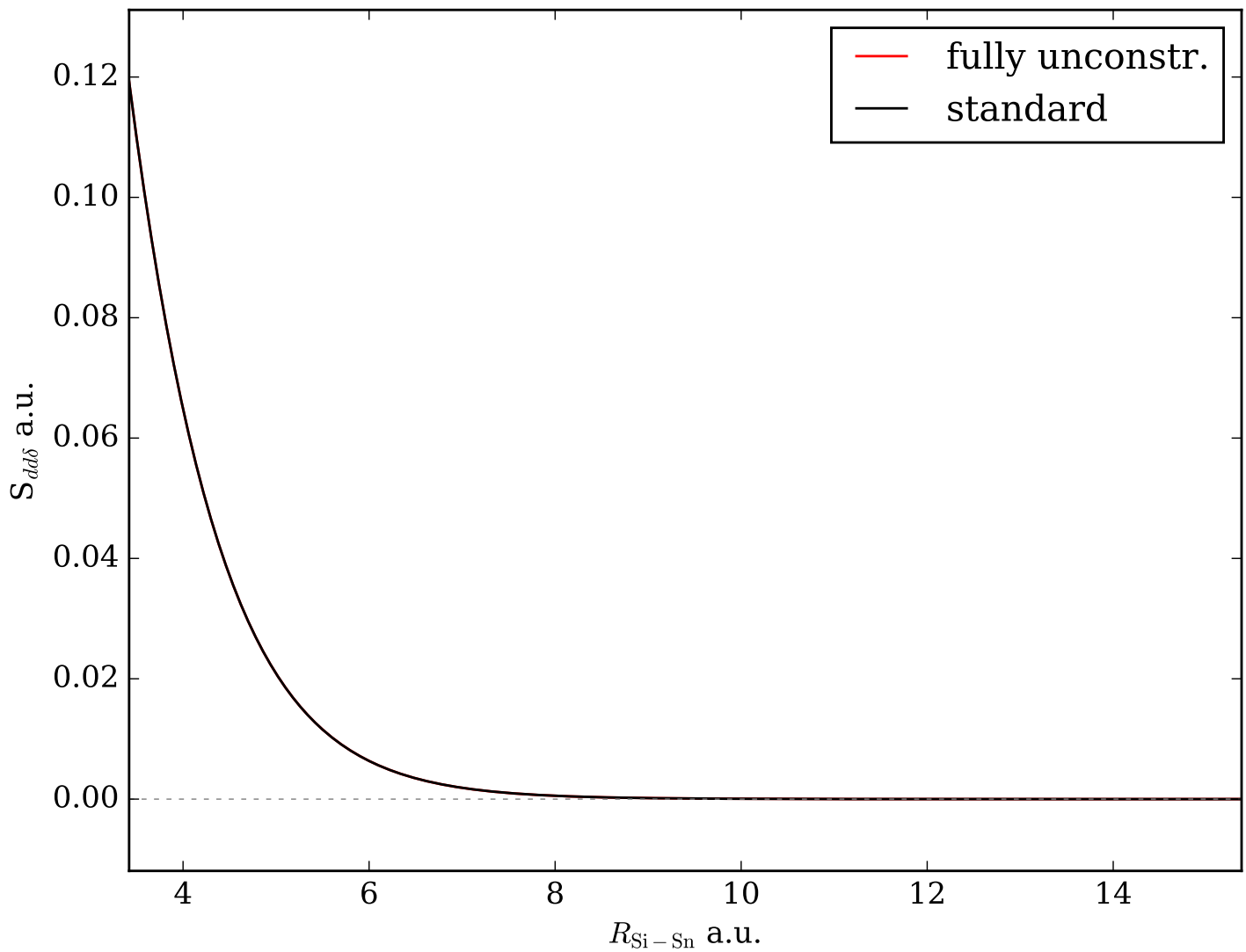
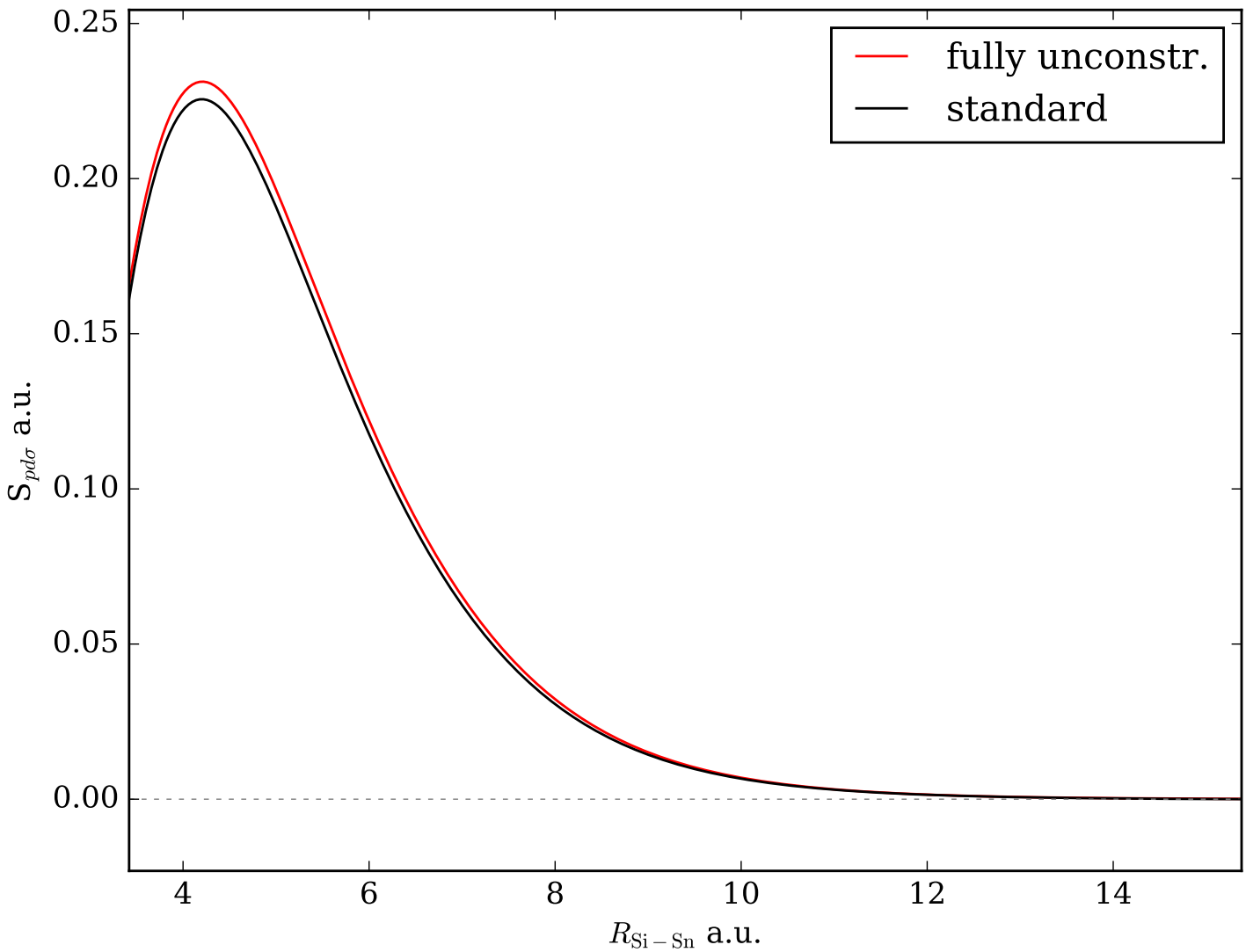
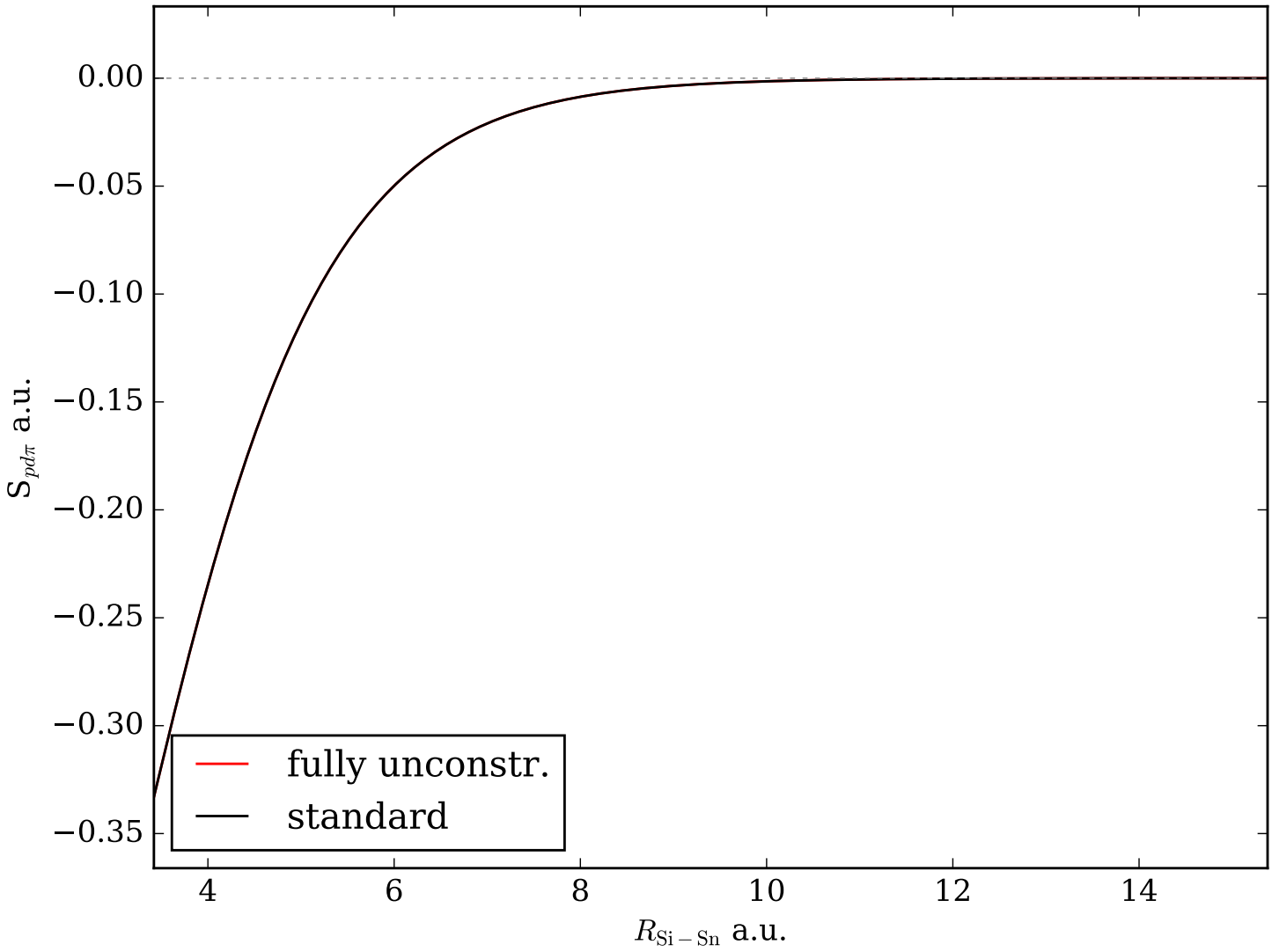
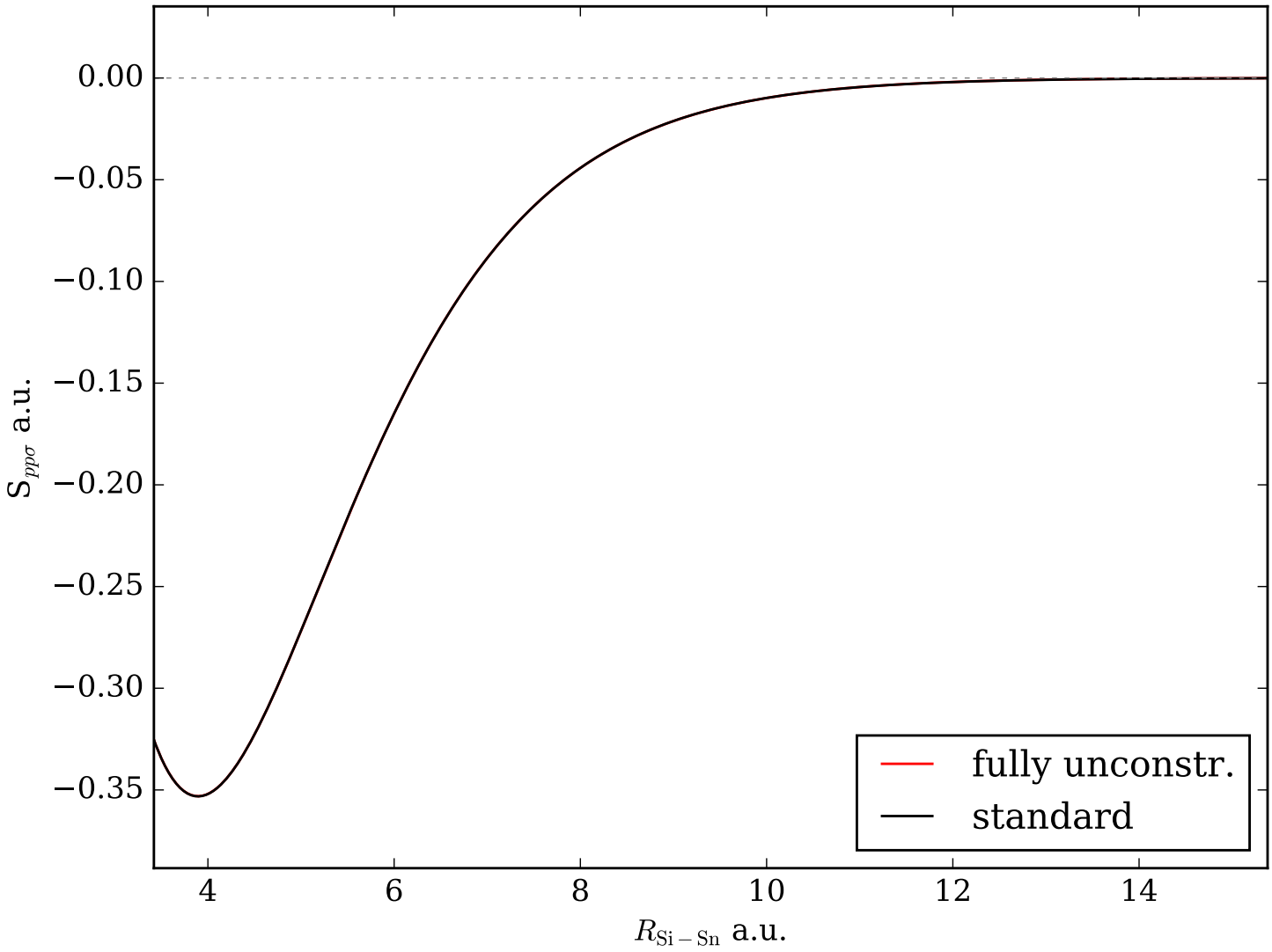
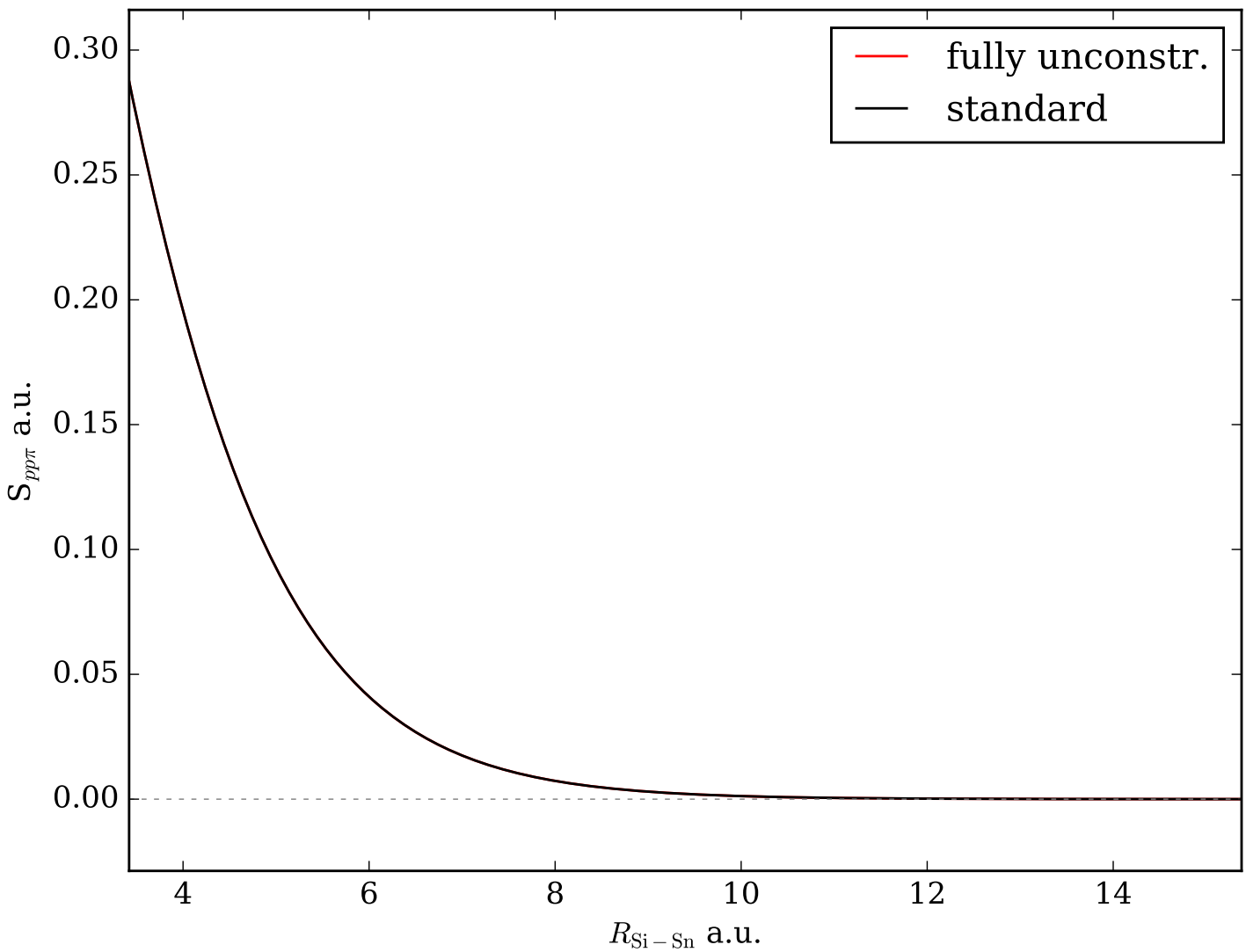
−0.1
−0.2
−0.3
−0.4
$S_{dd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.
fully unconstr.
standard

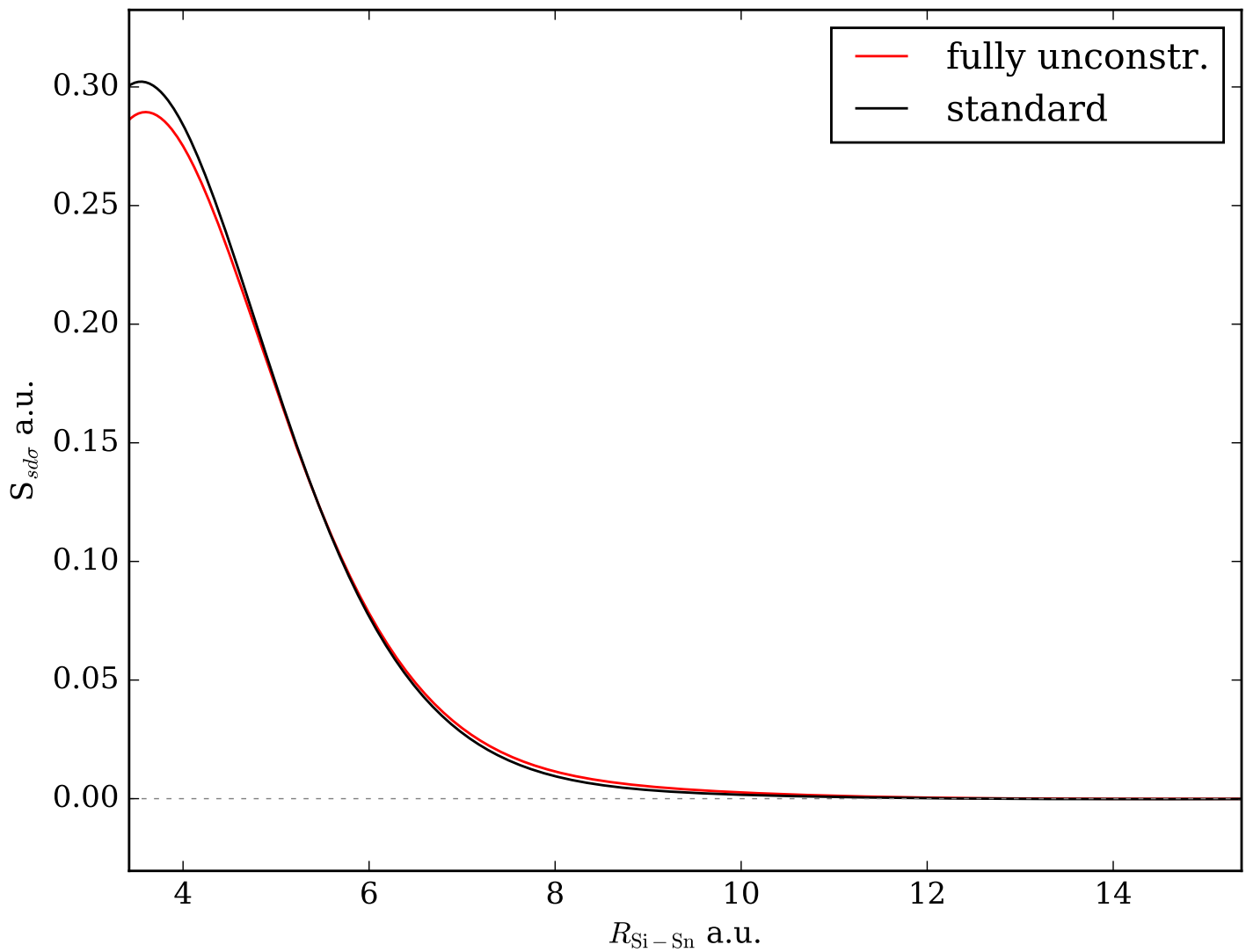

fully unconstr.
standard
0.12
0.10
0.08
0.06
0.04
0.02
0.00
$S_{dd\delta}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.

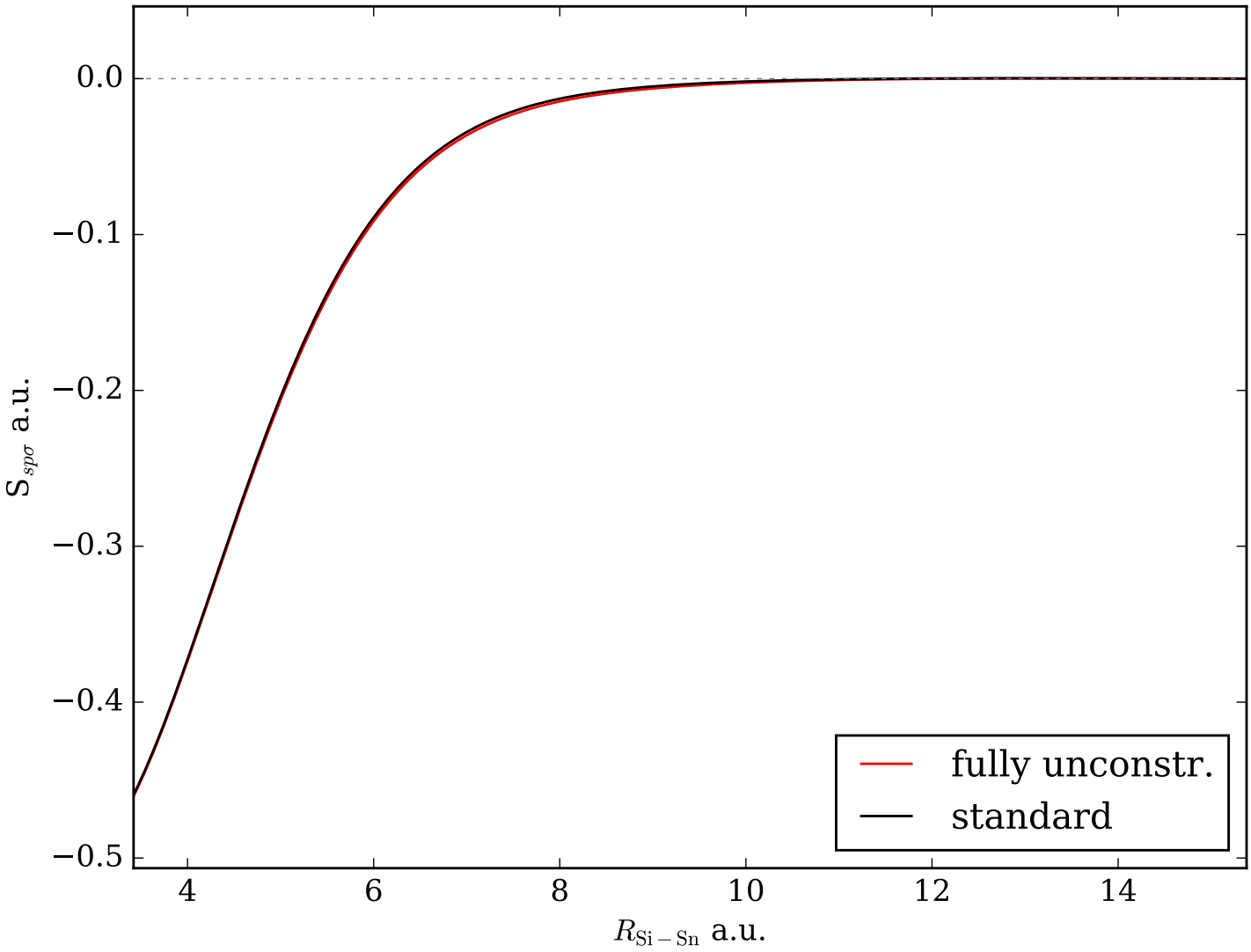

fully unconstr.
standard
0.25
0.20
0.15
0.10
0.05
0.00
$S_{pd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.

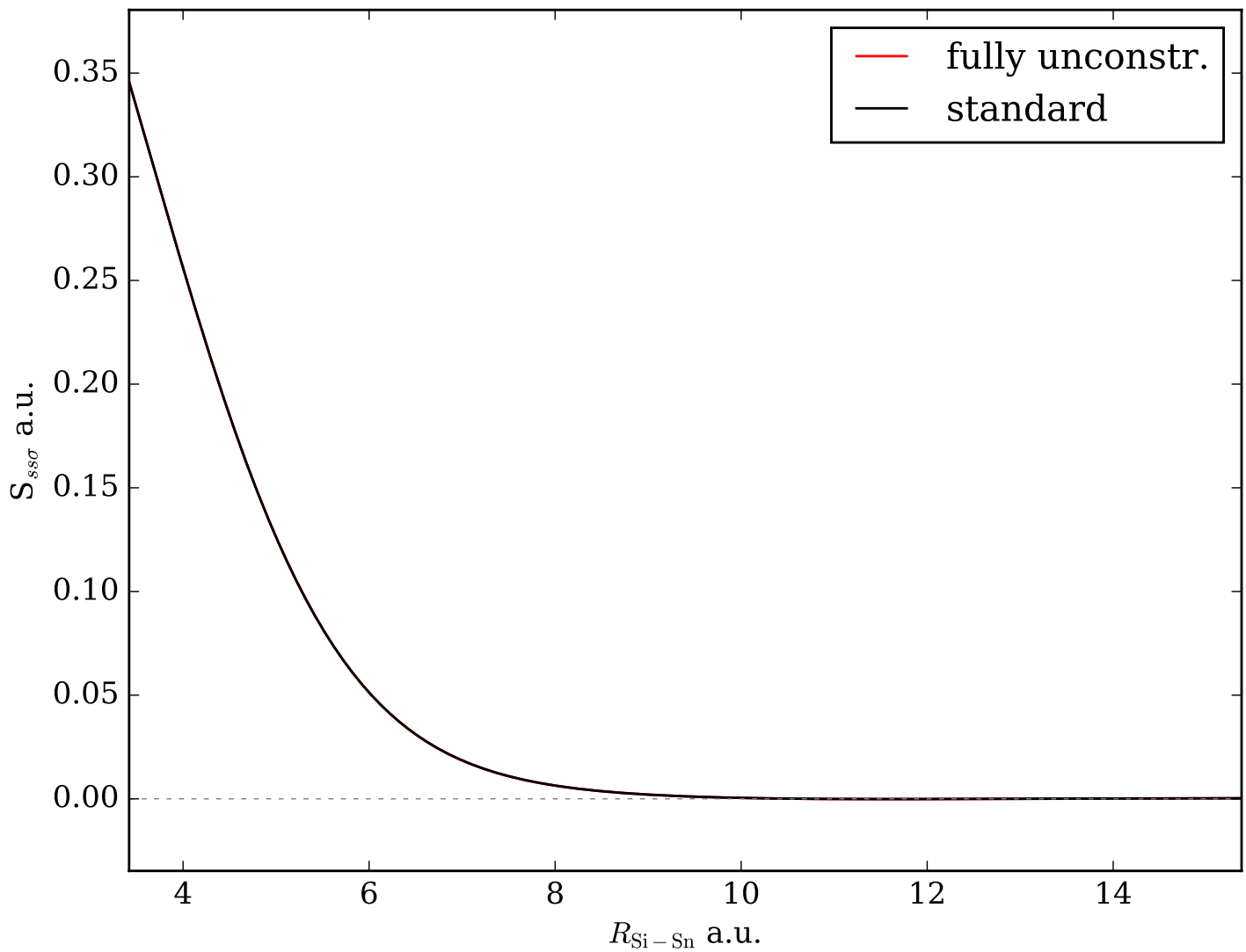

0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
−0.35
$S_{pd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.
fully unconstr.
standard


0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
−0.35
$S_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.
fully unconstr.
standard

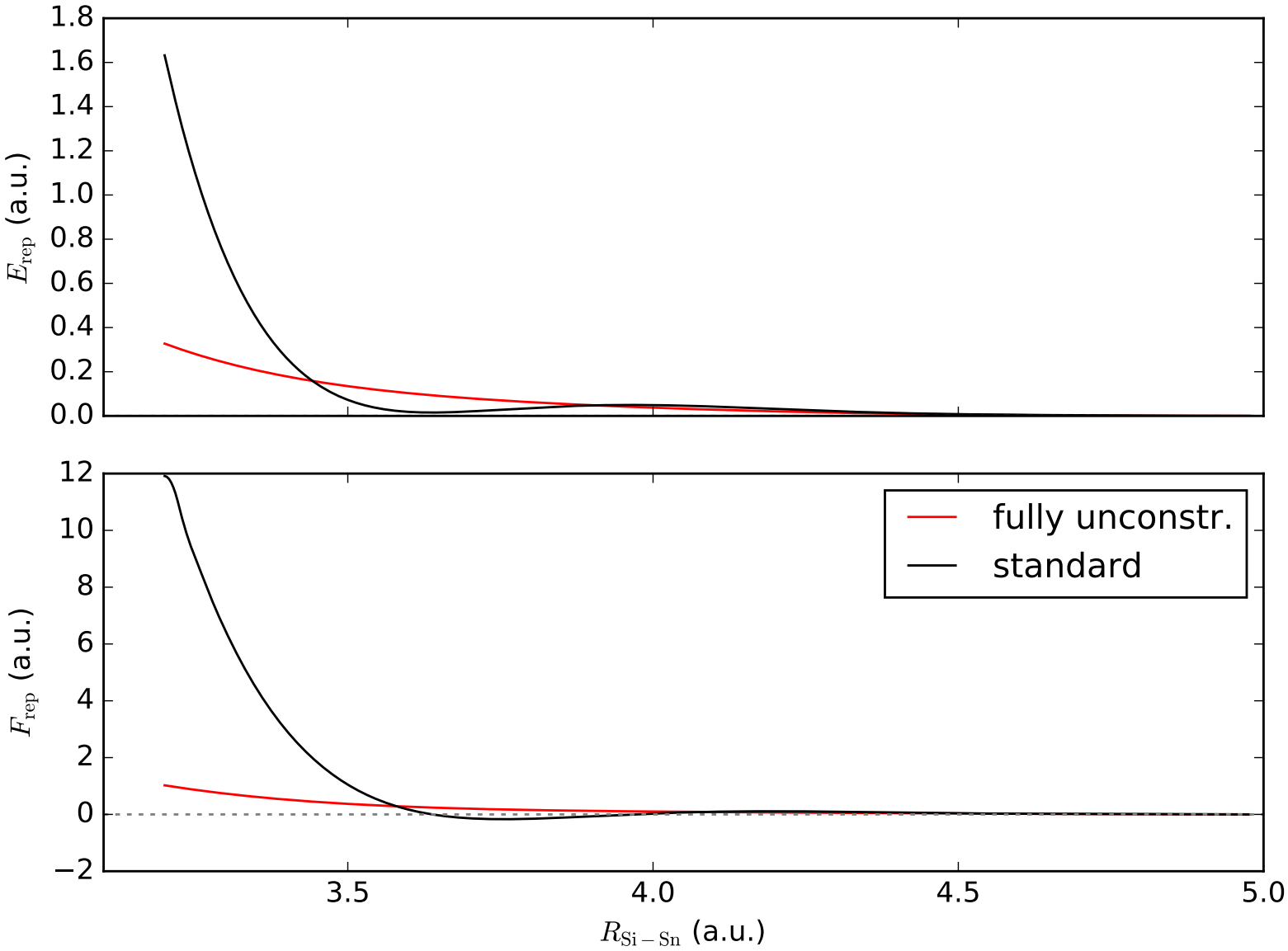

fully unconstr.
standard
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$S_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.


fully unconstr.
standard
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$S_{sd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.


0.0
−0.1
−0.2
−0.3
−0.4
−0.5
$S_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.
fully unconstr.
standard

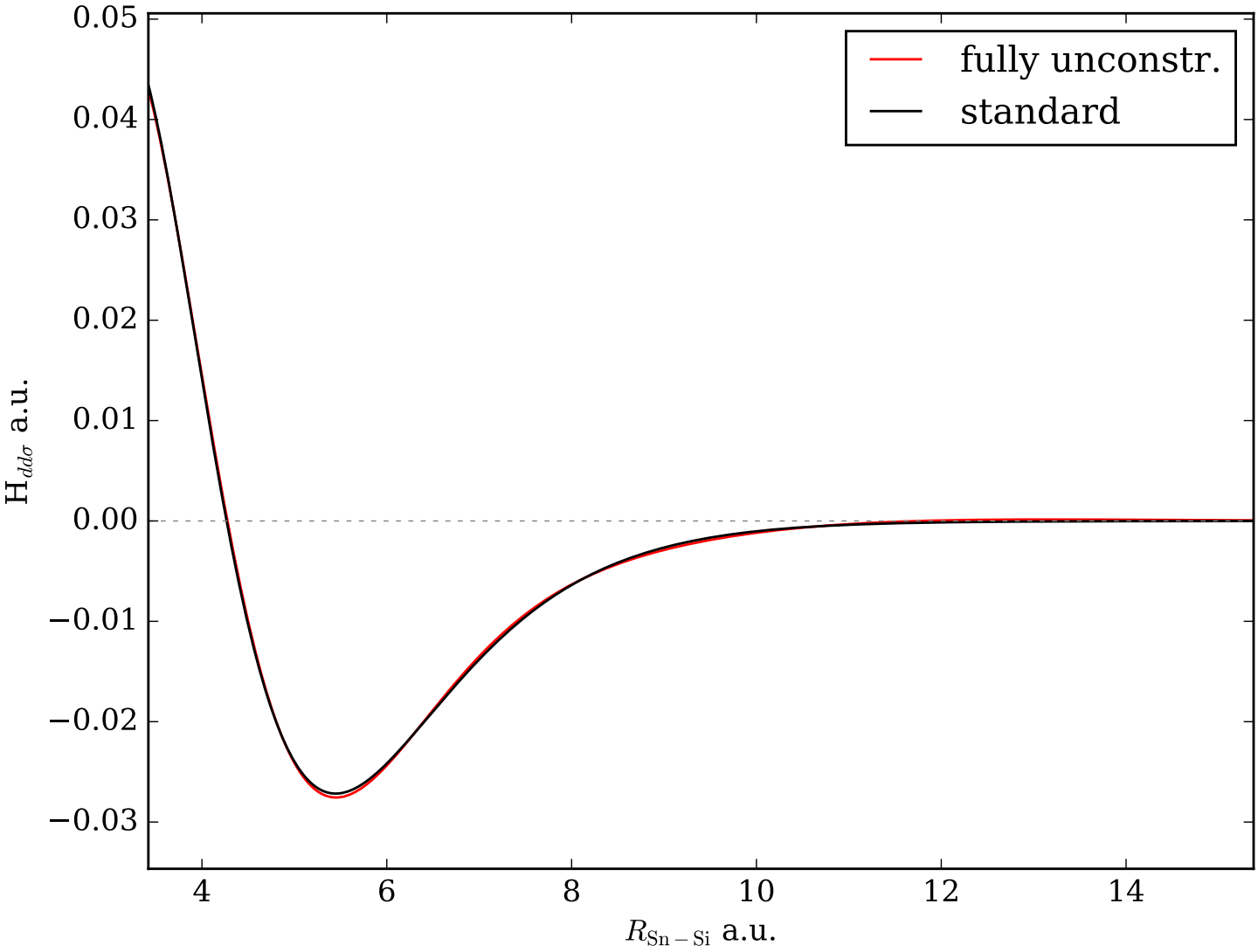

fully unconstr.
standard
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$S_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Si-Sn}}$ a.u.

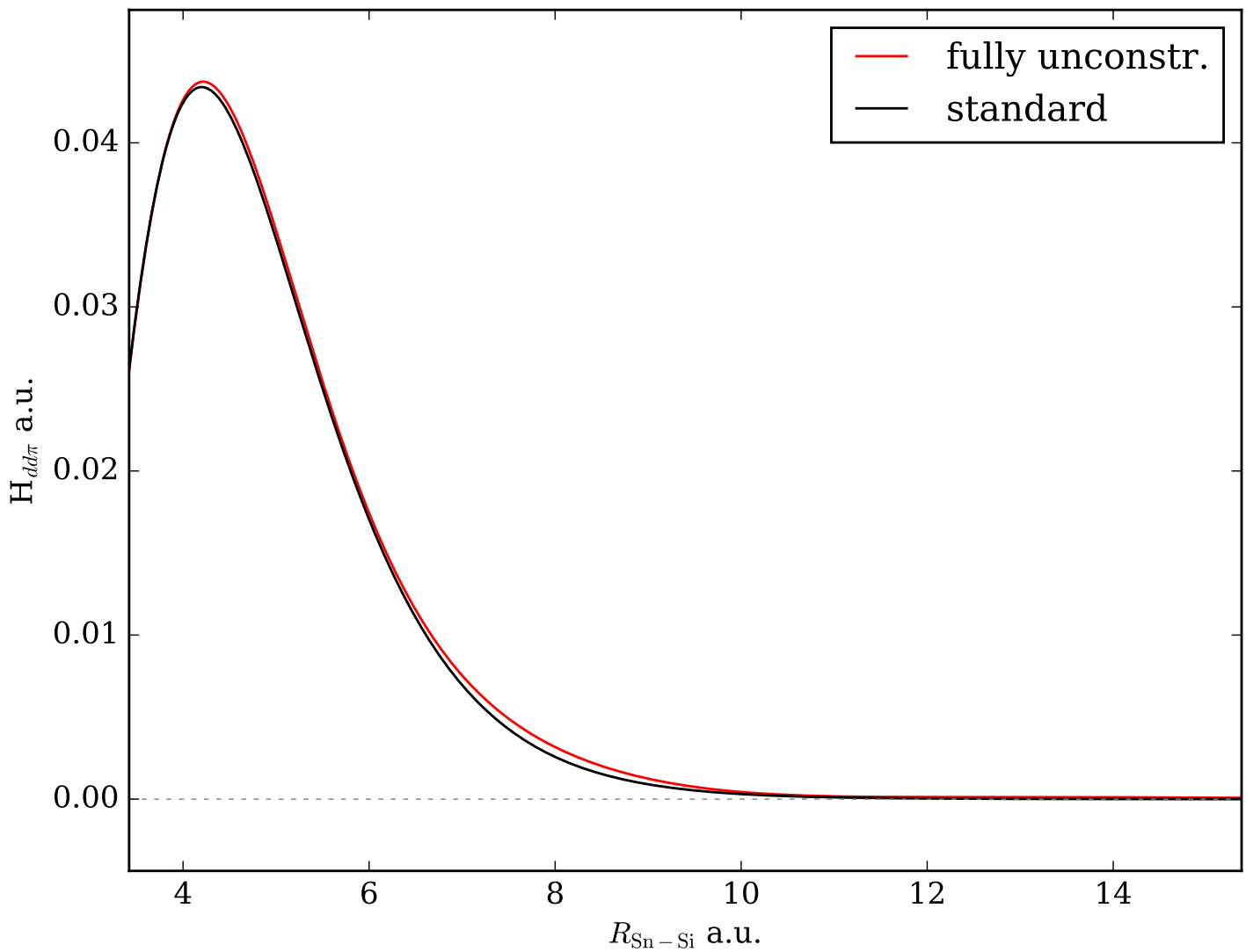
13.2 Repulsive

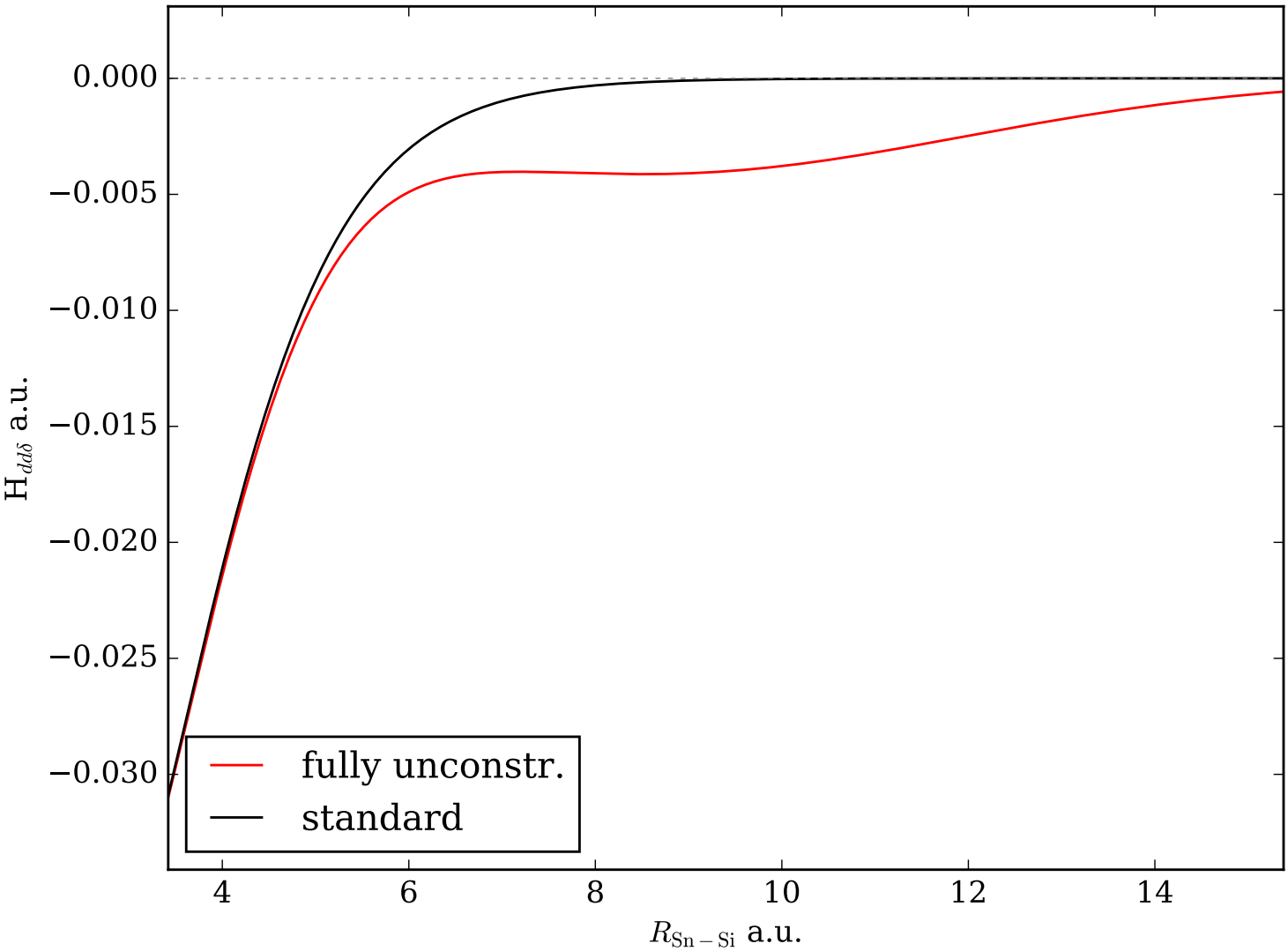


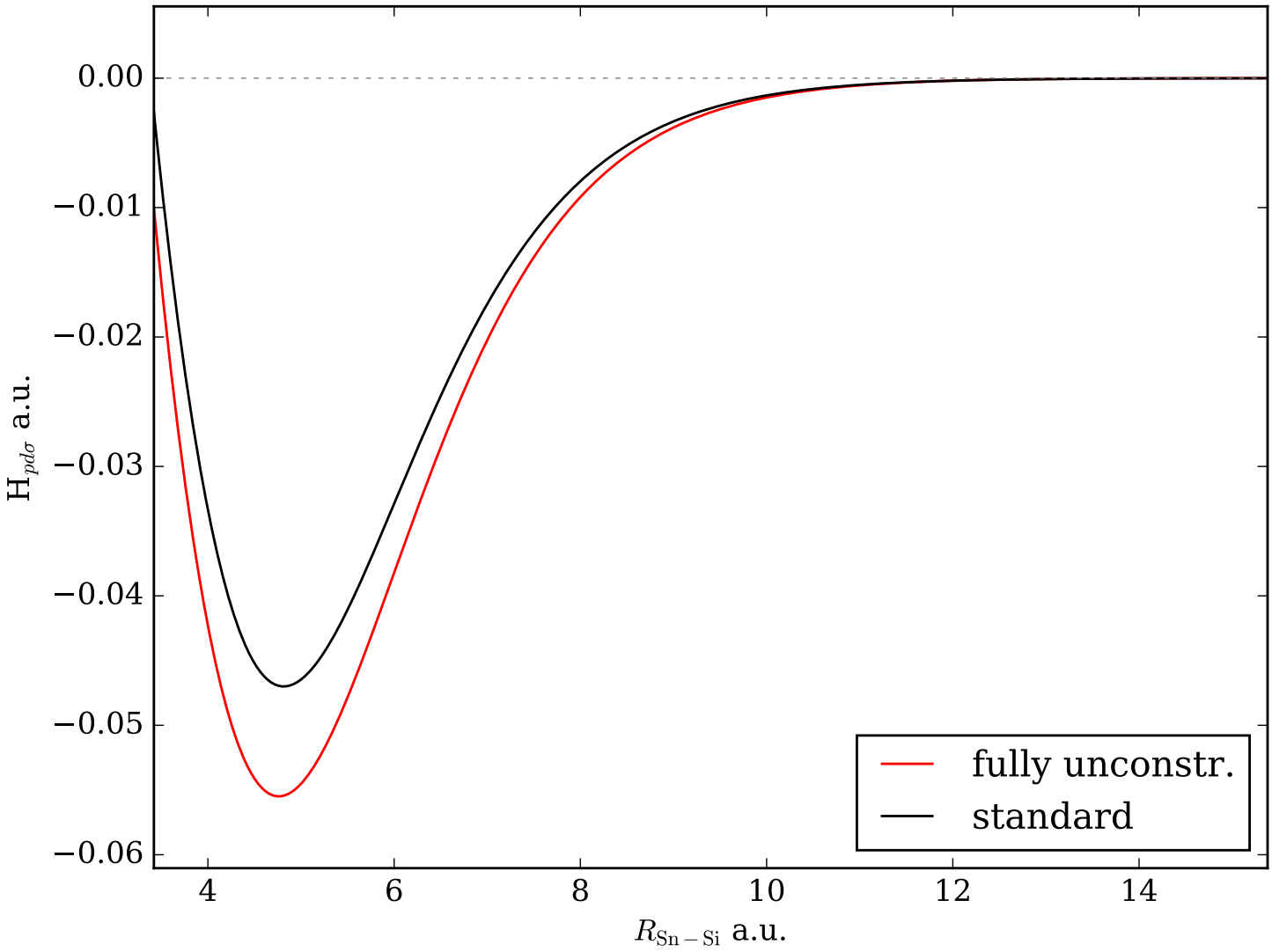
14 Sn-Si

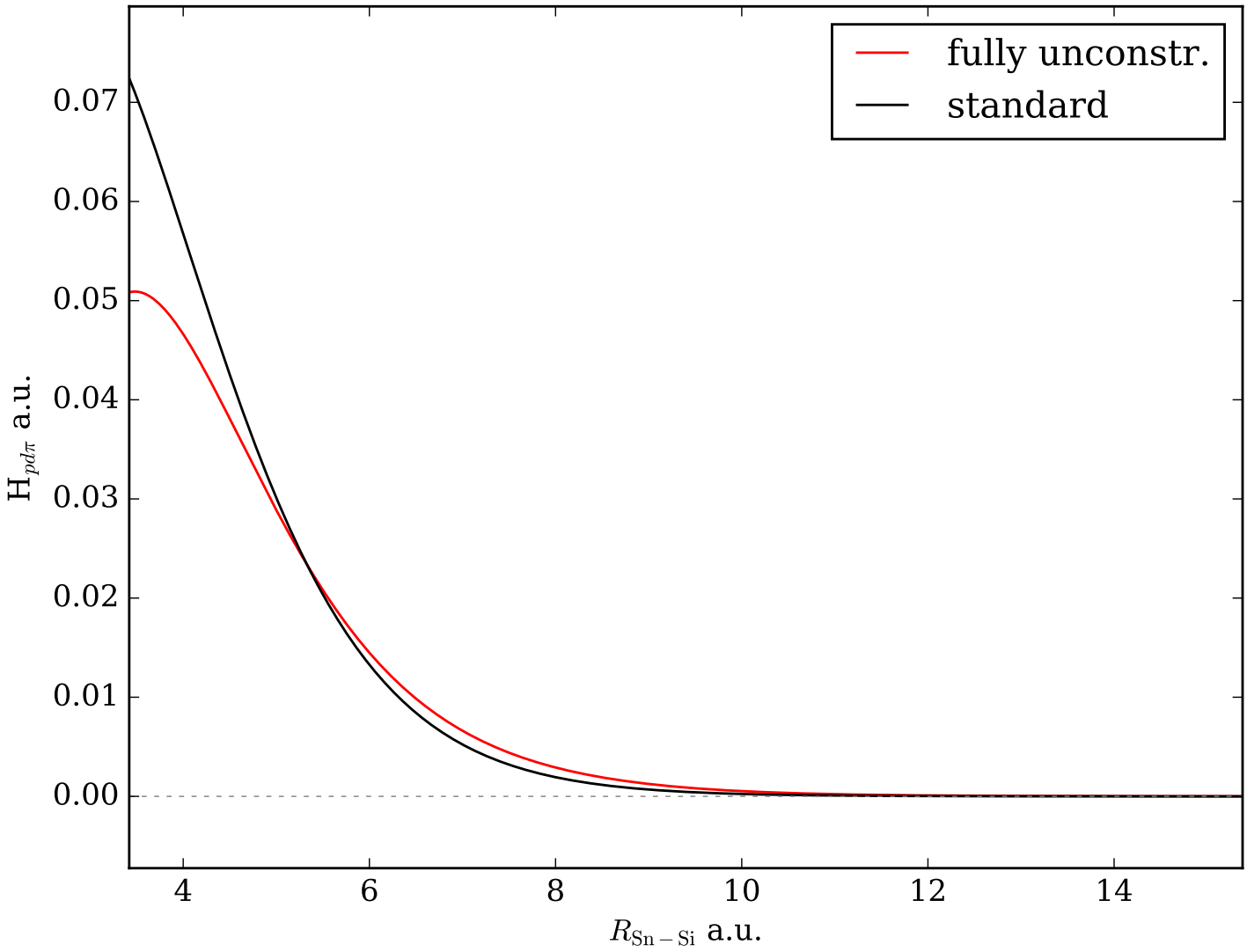
14.1 Electronic




fully unconstr.
standard
0.04
0.03
0.02
0.01
0.00
$H_{dd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.


0.000
−0.005
−0.010
−0.015
−0.020
−0.025
−0.030
$H_{dd\delta}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.
fully unconstr.
standard


0.00
−0.01
−0.02
−0.03
−0.04
−0.05
−0.06
$H_{pd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.
fully unconstr.
standard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standard
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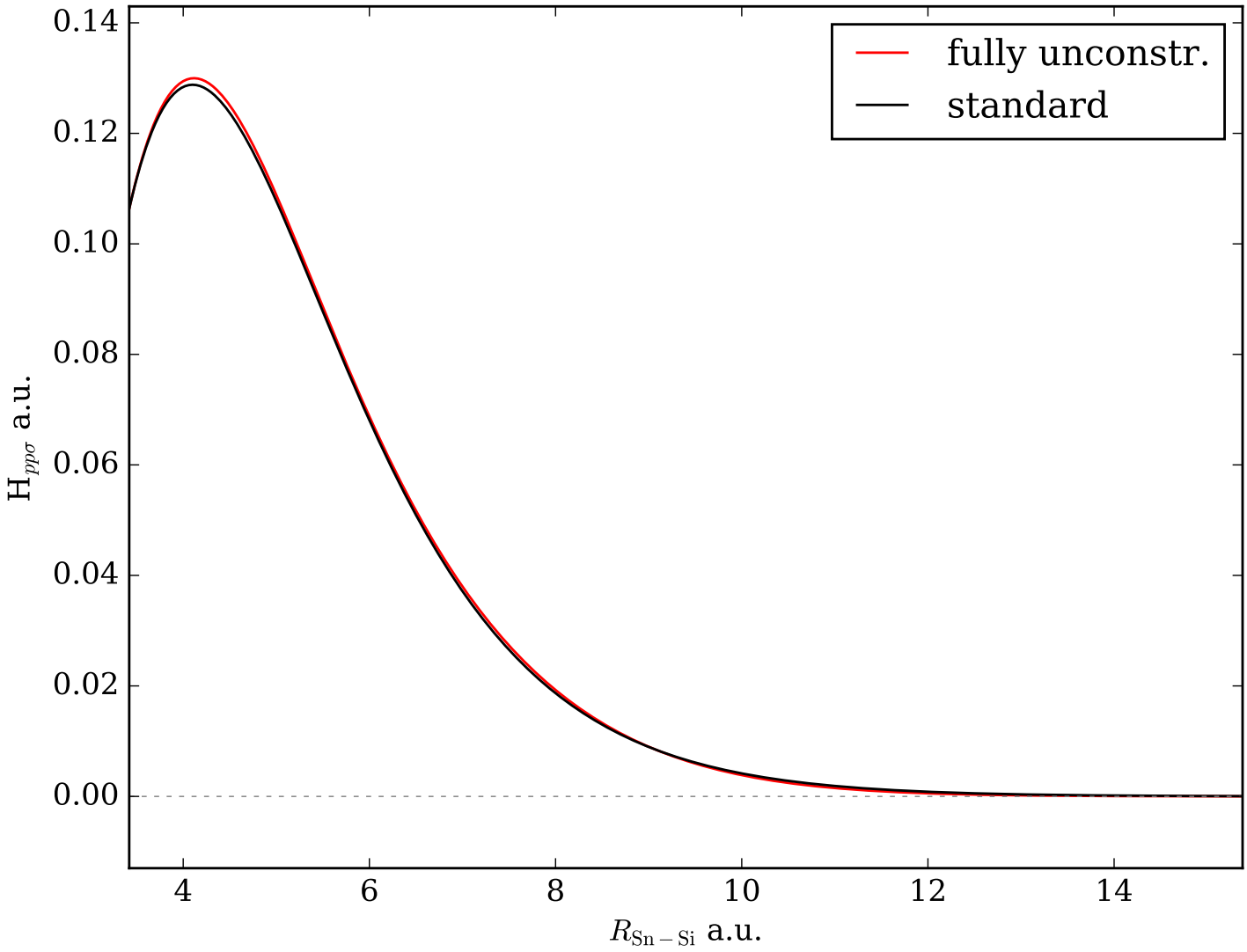
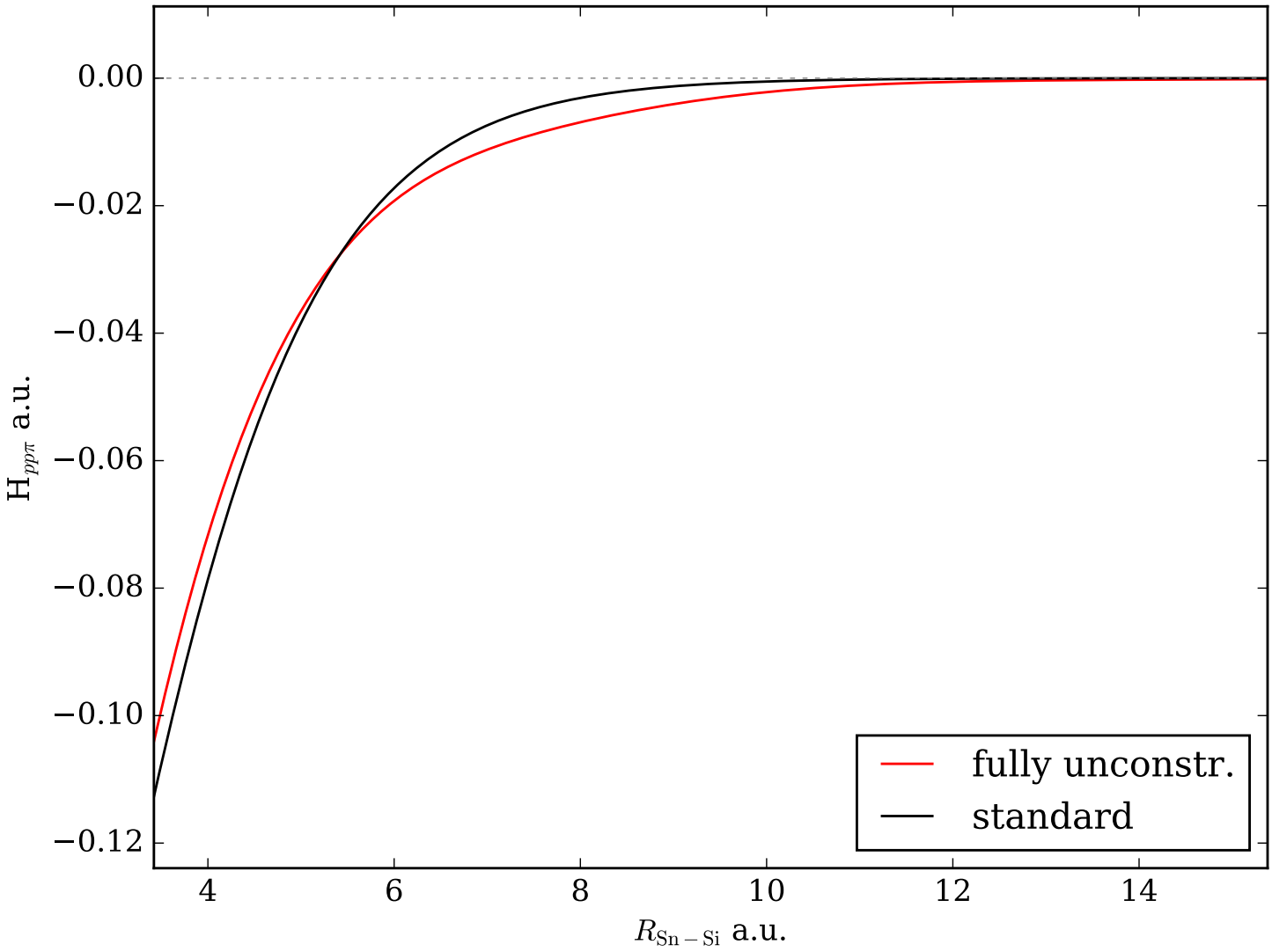
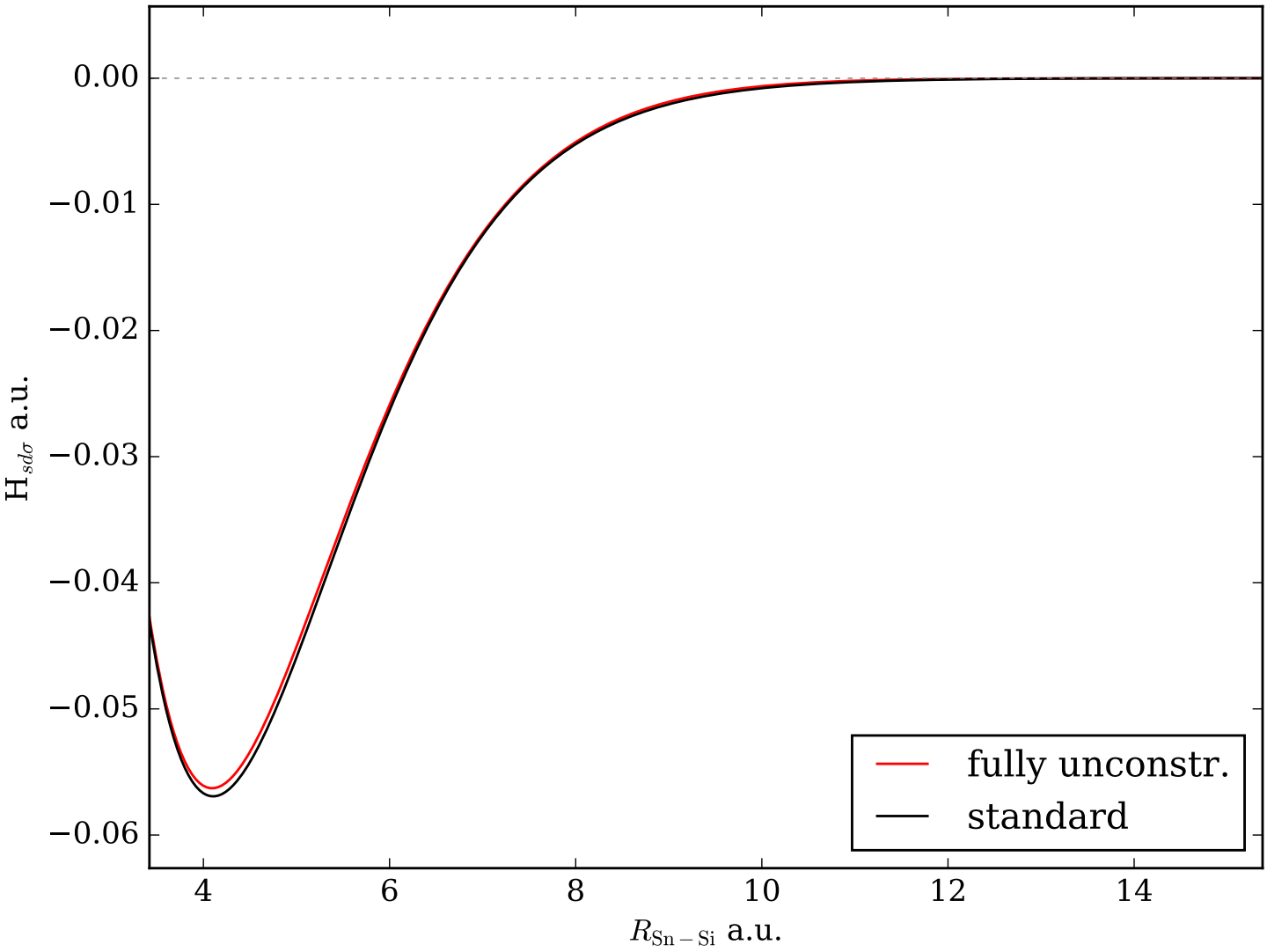
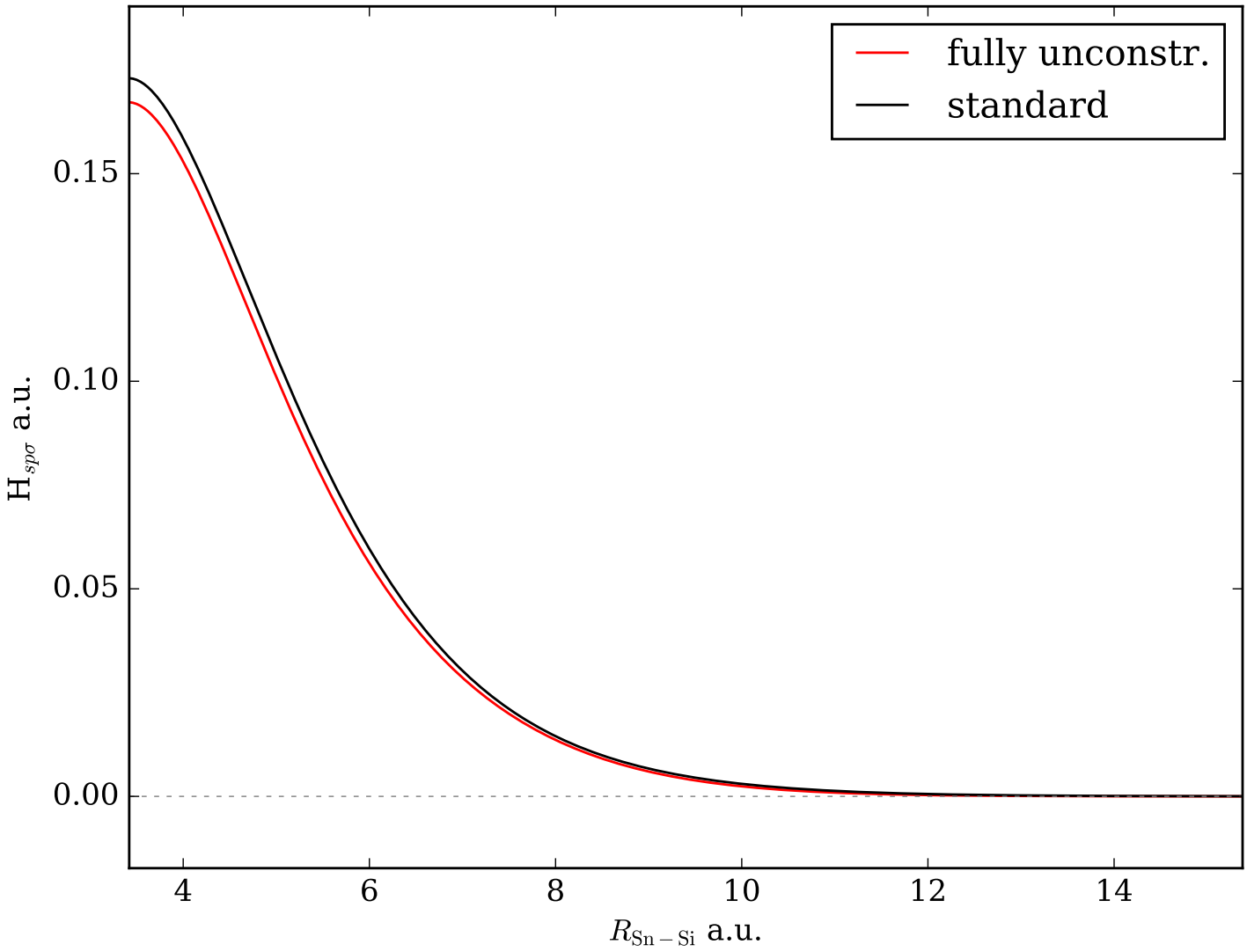
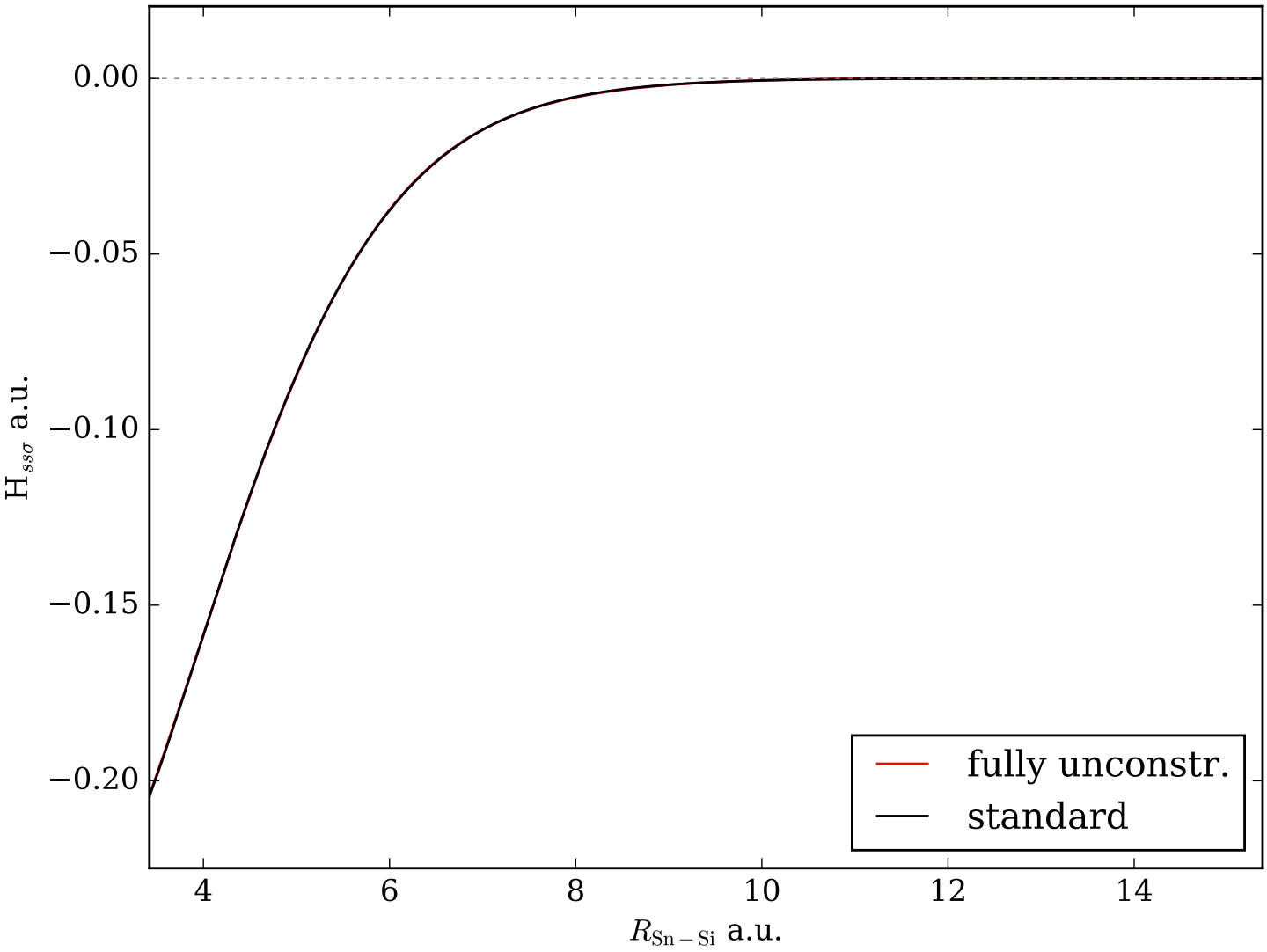
0.06
0.05
0.04
0.03
0.02
0.01
0.00
$H_{pd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.


fully unconstr.
standard
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
$H_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.


0.00
−0.02
−0.04
−0.06
−0.08
−0.10
−0.12
$H_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.
fully unconstr.
standard


0.00
−0.01
−0.02
−0.03
−0.04
−0.05
−0.06
$H_{sd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.15
0.10
0.05
0.00
$H_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.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−0.05
−0.10
−0.15
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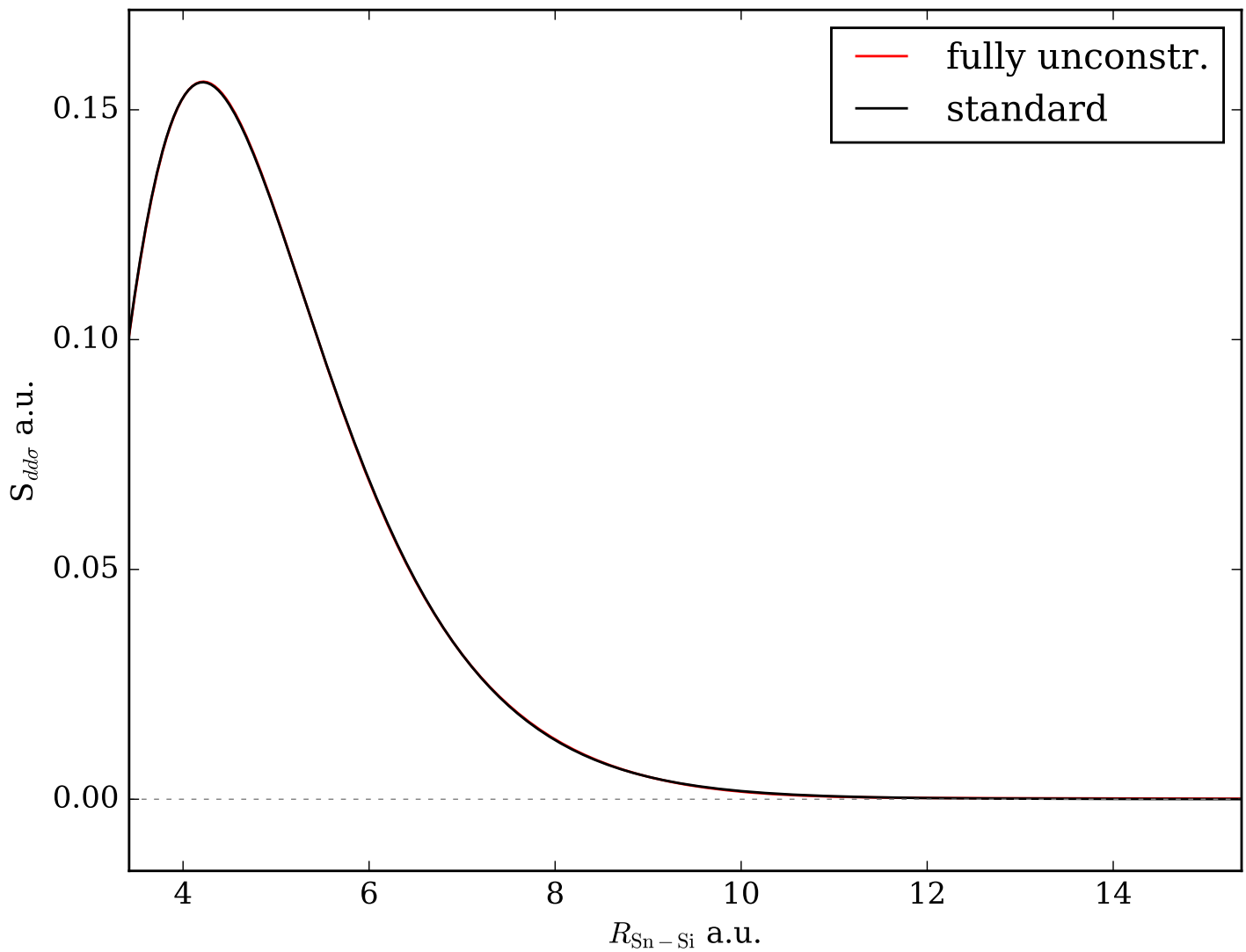
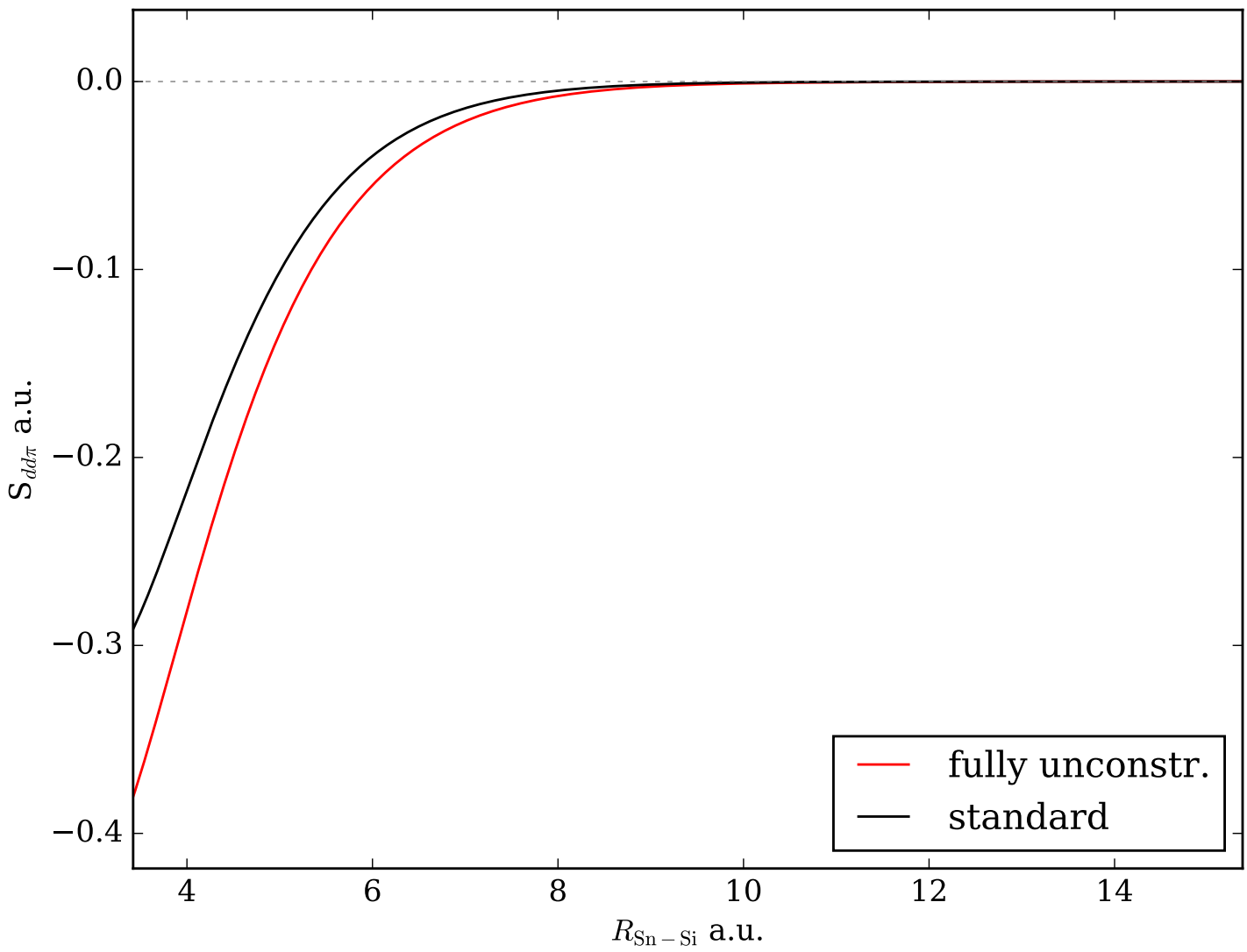
$H_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.15
0.10
0.05
0.00
$S_{dd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.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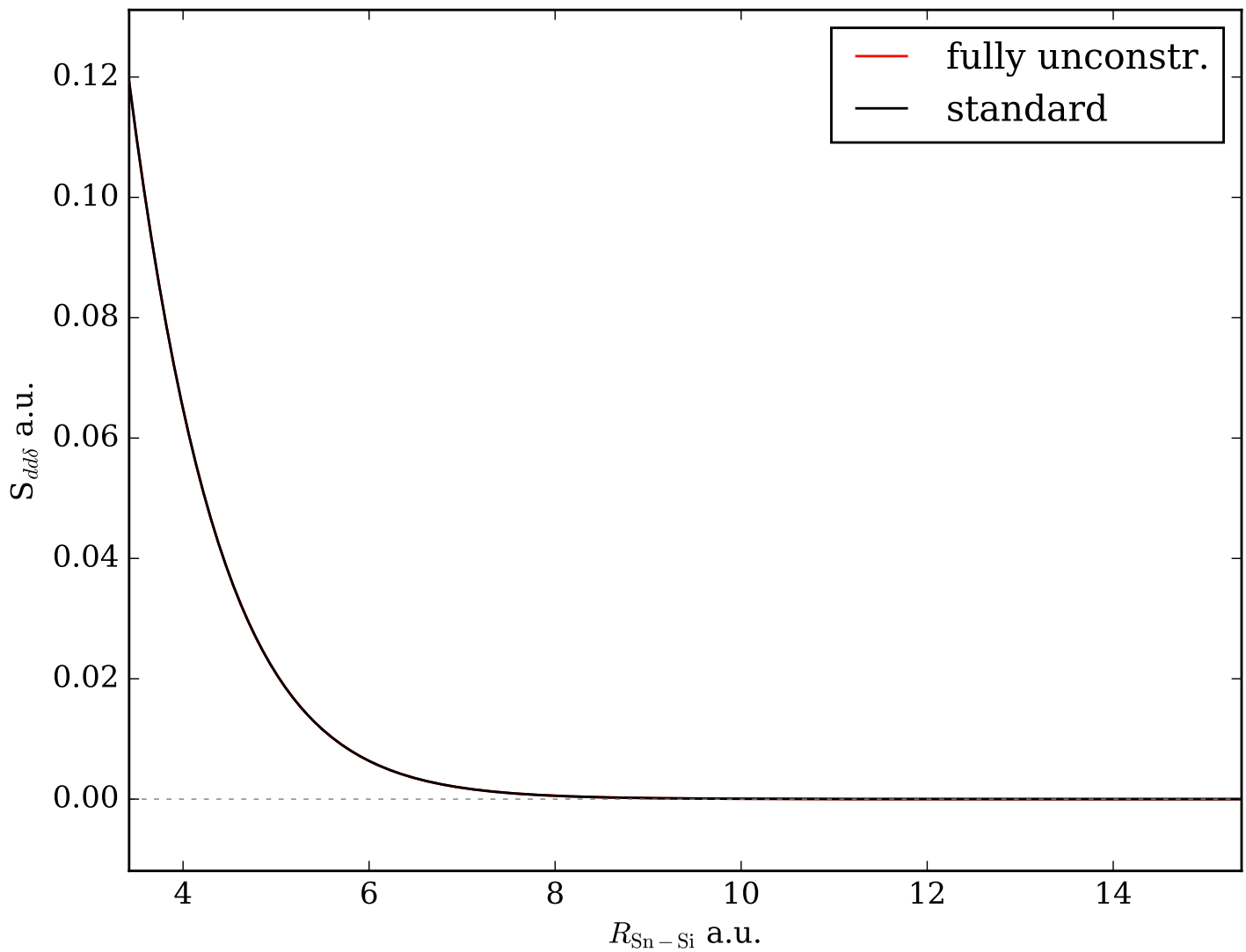
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
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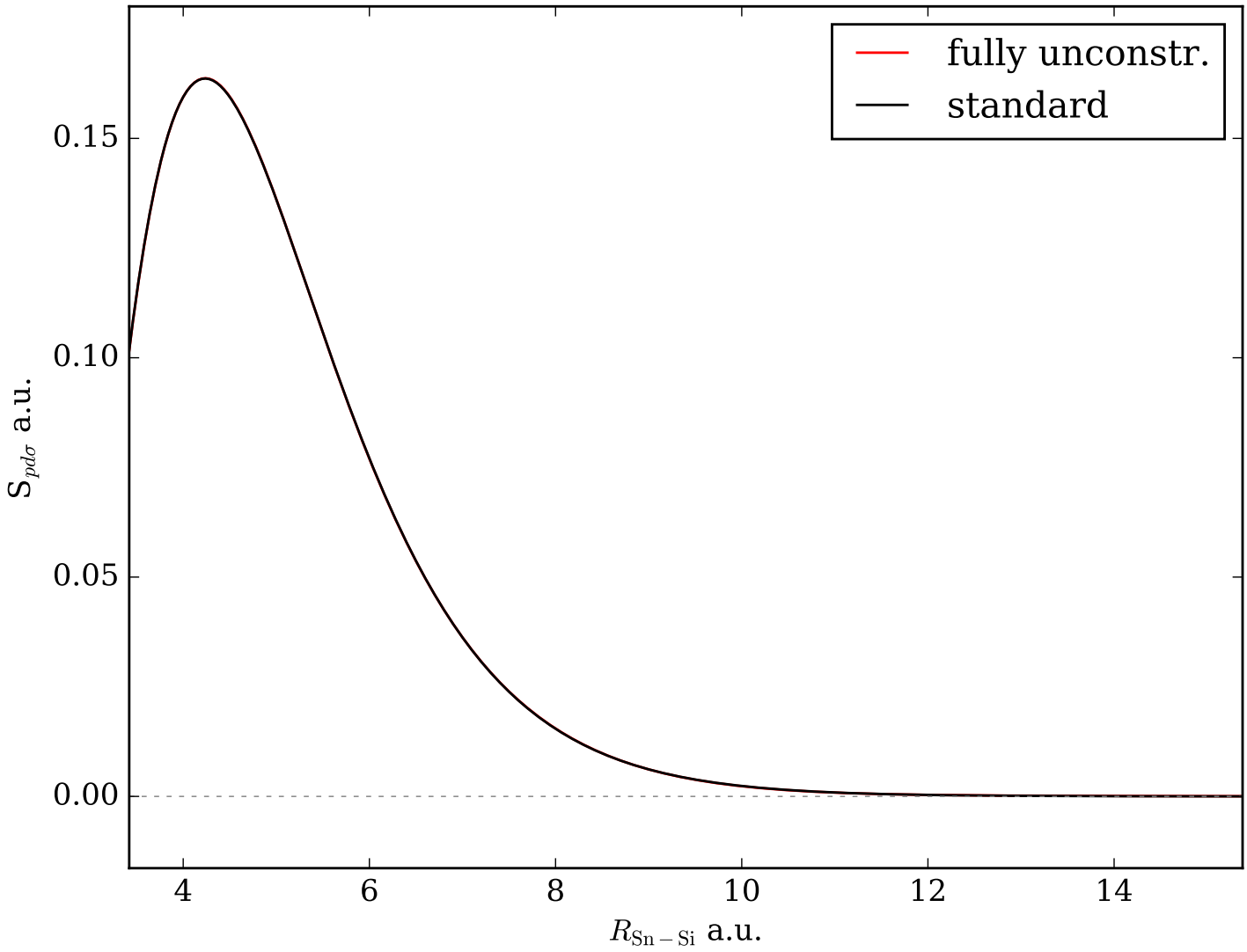
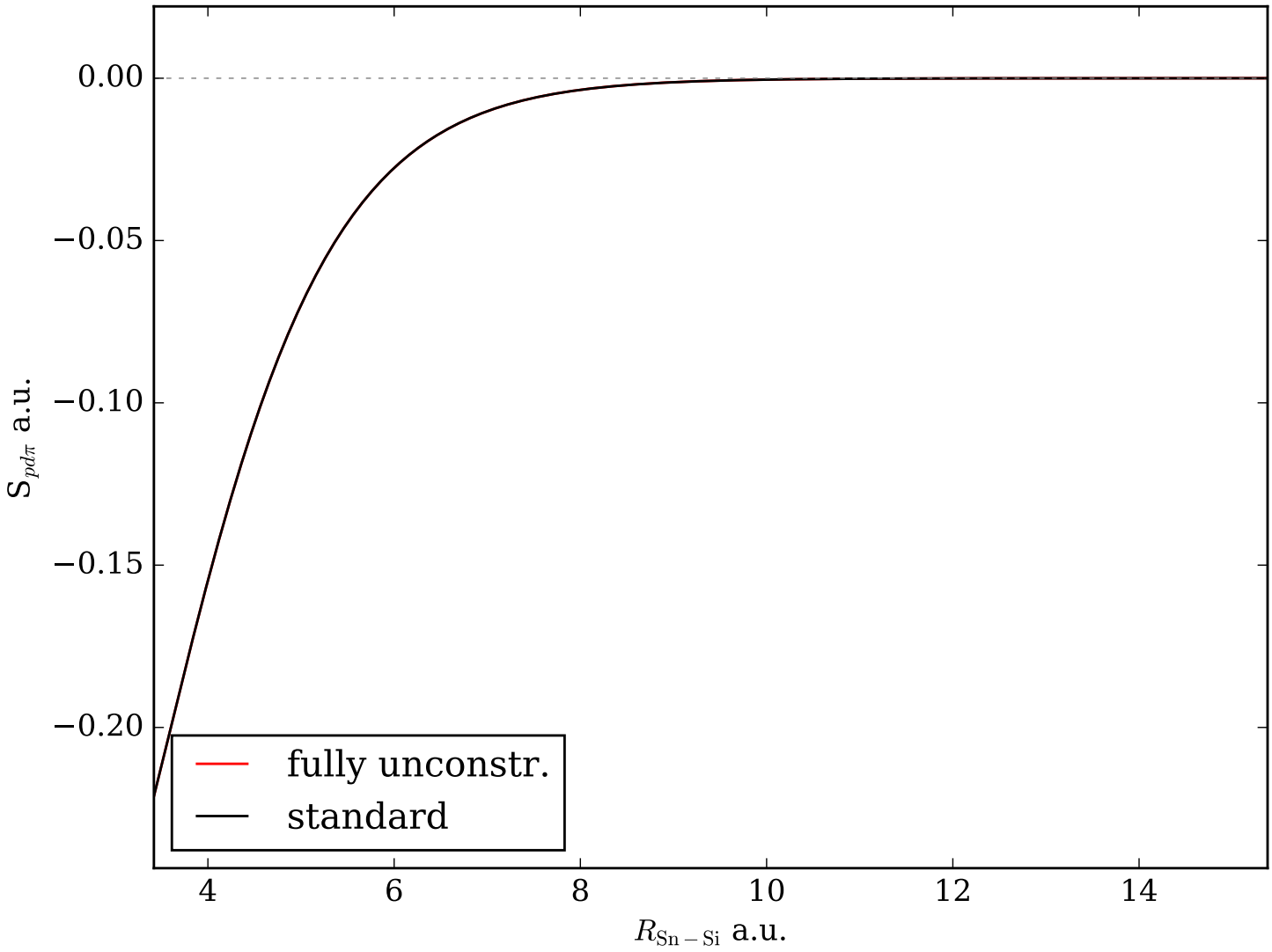
0.10
0.08
0.06
0.04
0.02
0.00
$S_{dd\delta}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.


fully unconstr.
standard
0.15
0.10
0.05
0.00
$S_{pd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.


0.00
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−0.10
−0.15
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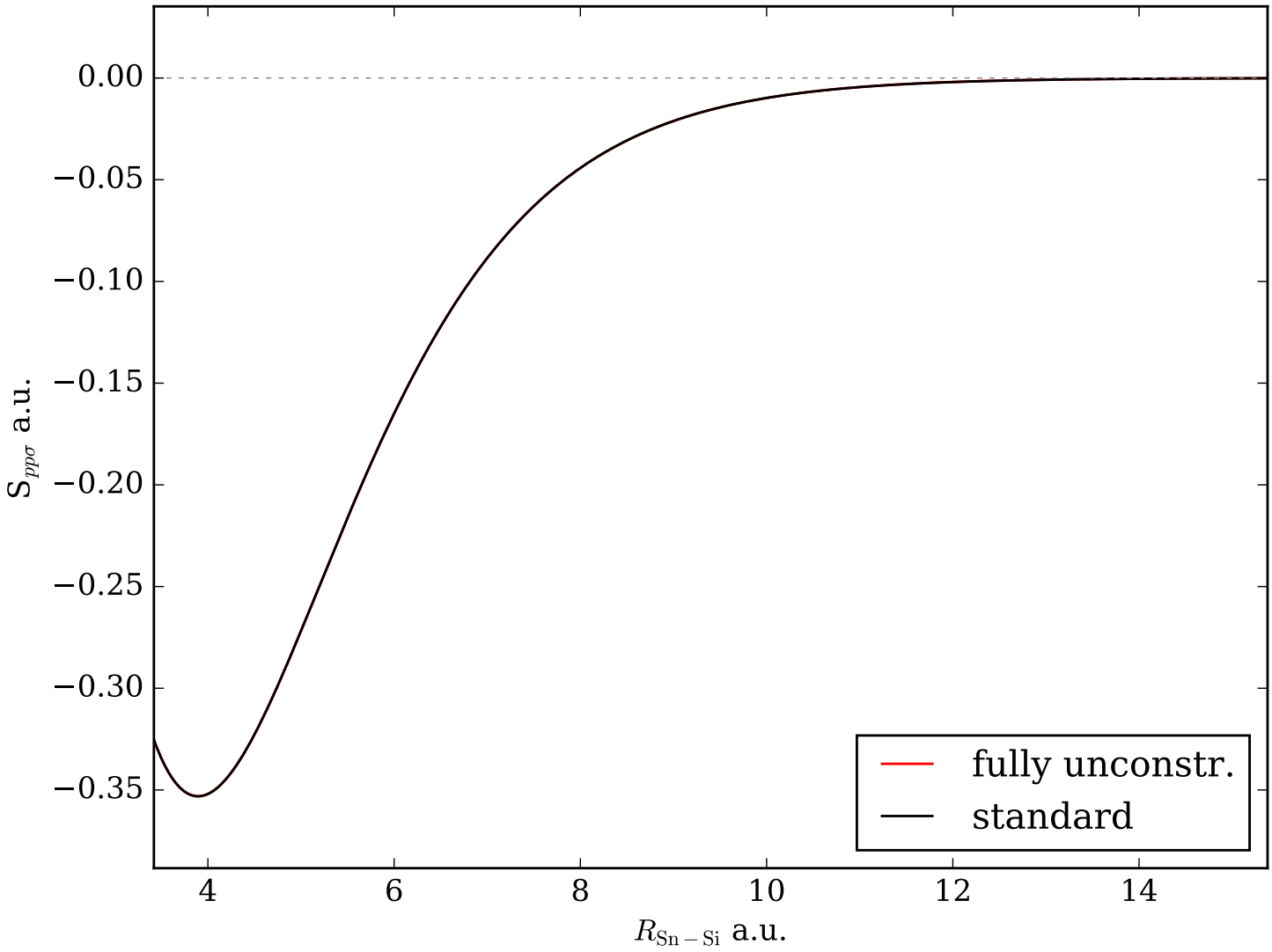
$S_{pd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.
fully unconstr.
standard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−0.10
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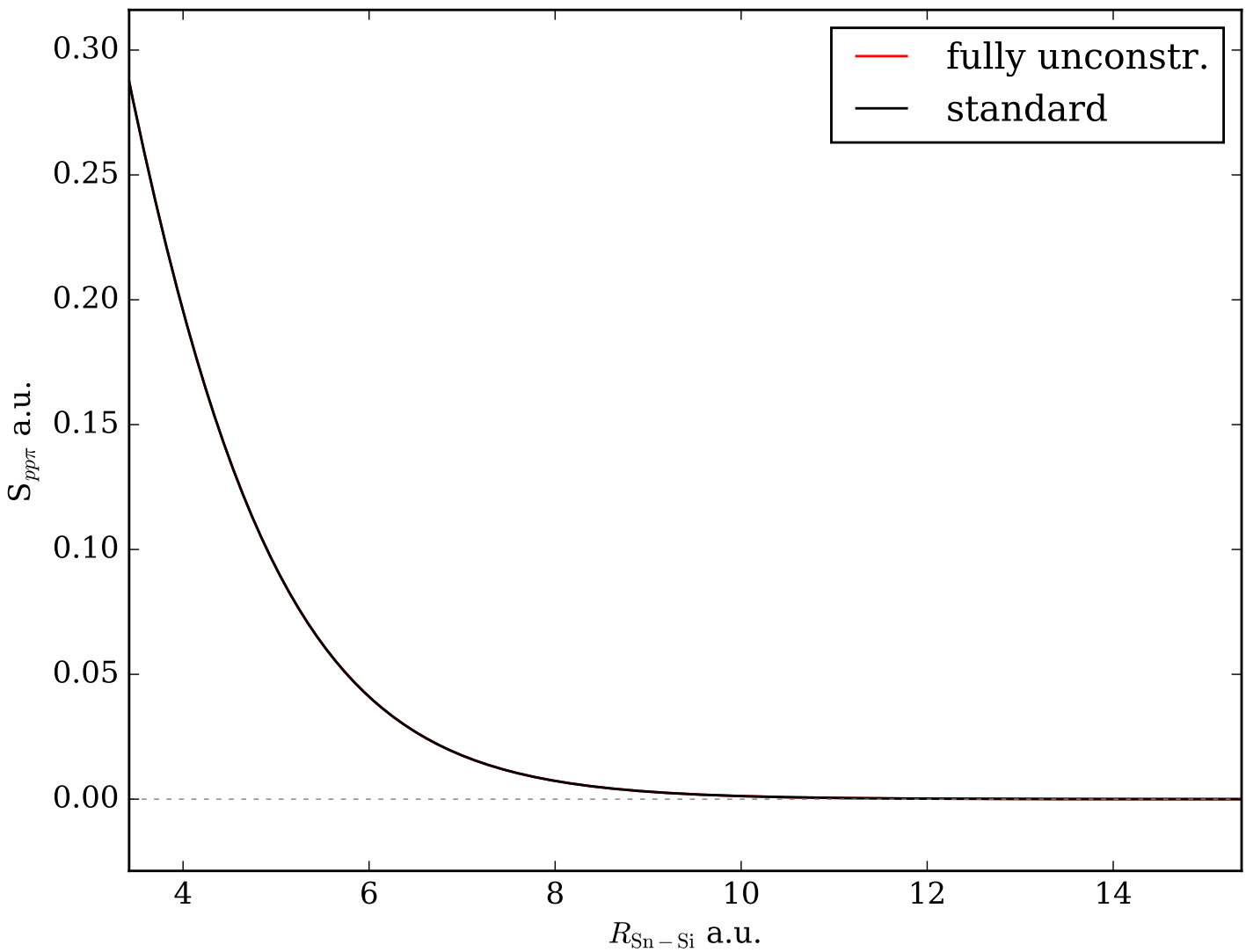
−0.30
−0.35
$S_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
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0.25
0.20
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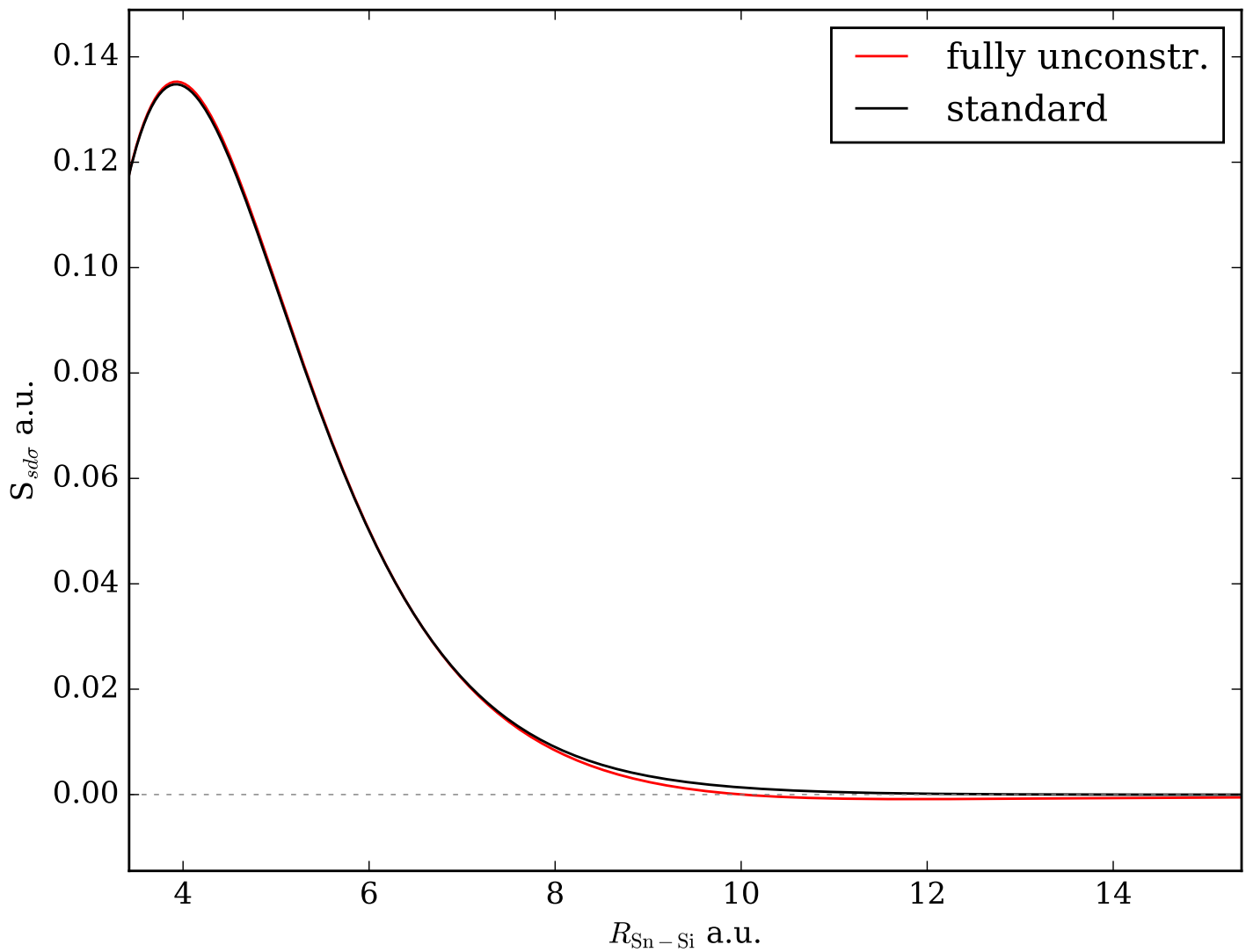
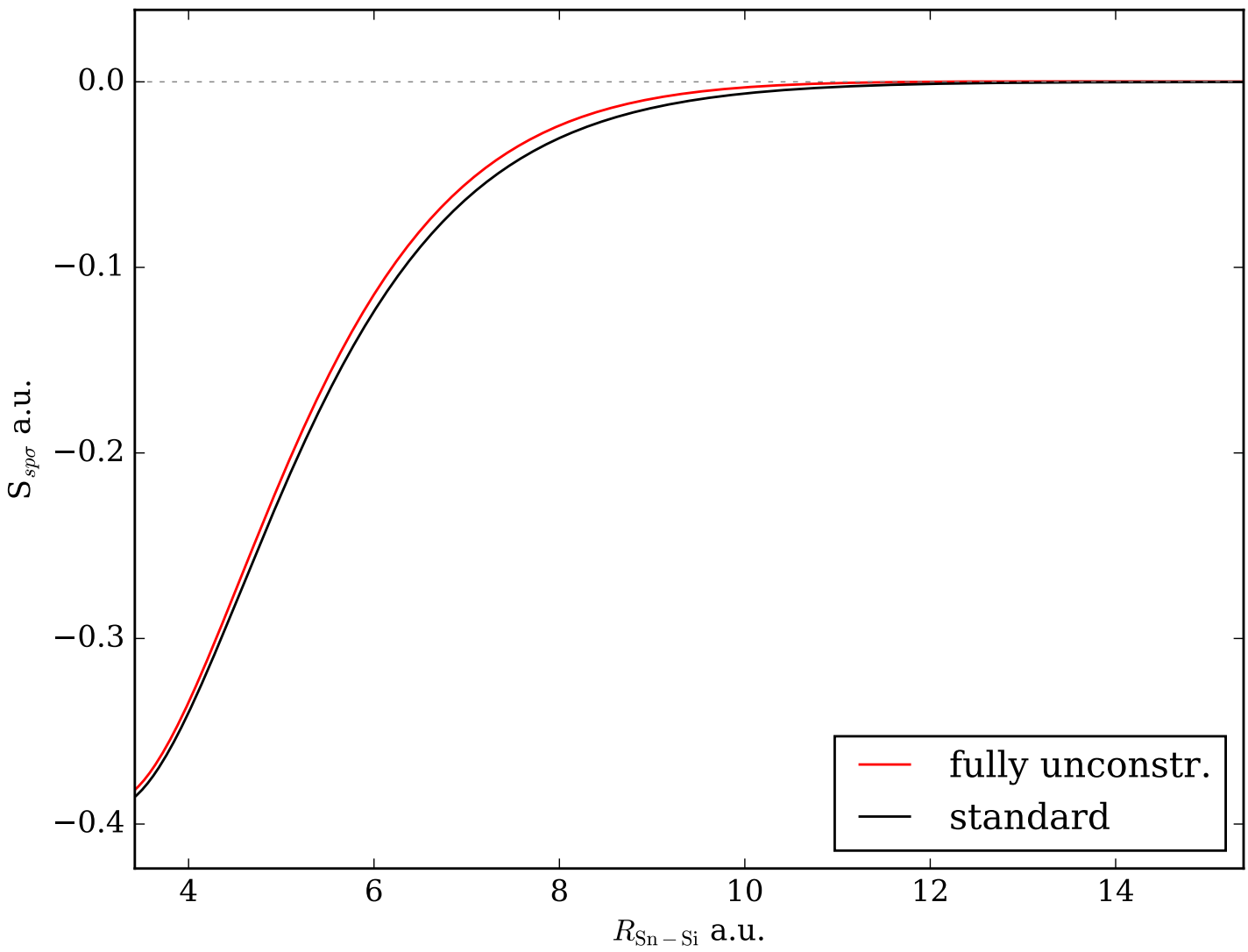
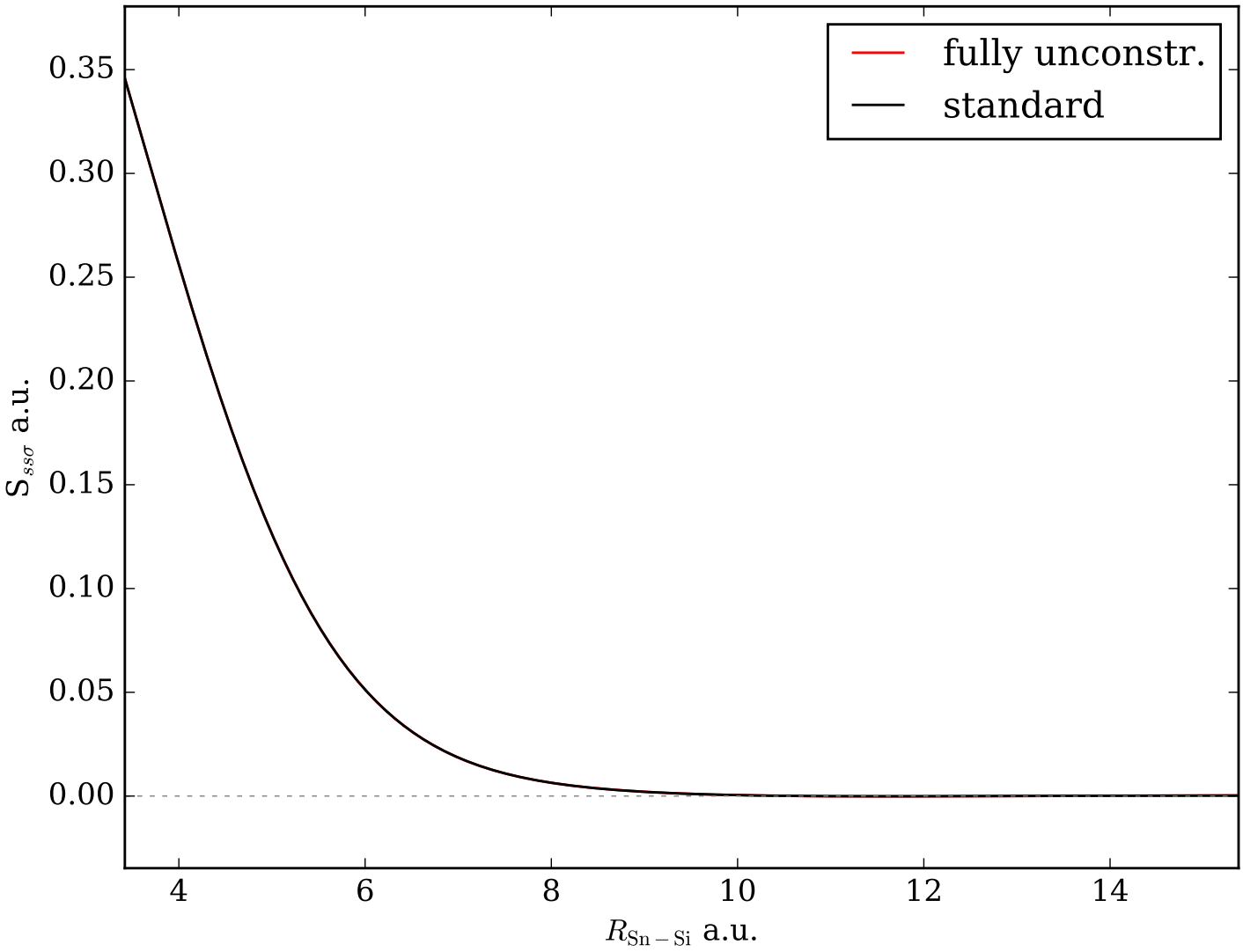
0.10
0.05
0.00
$S_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.

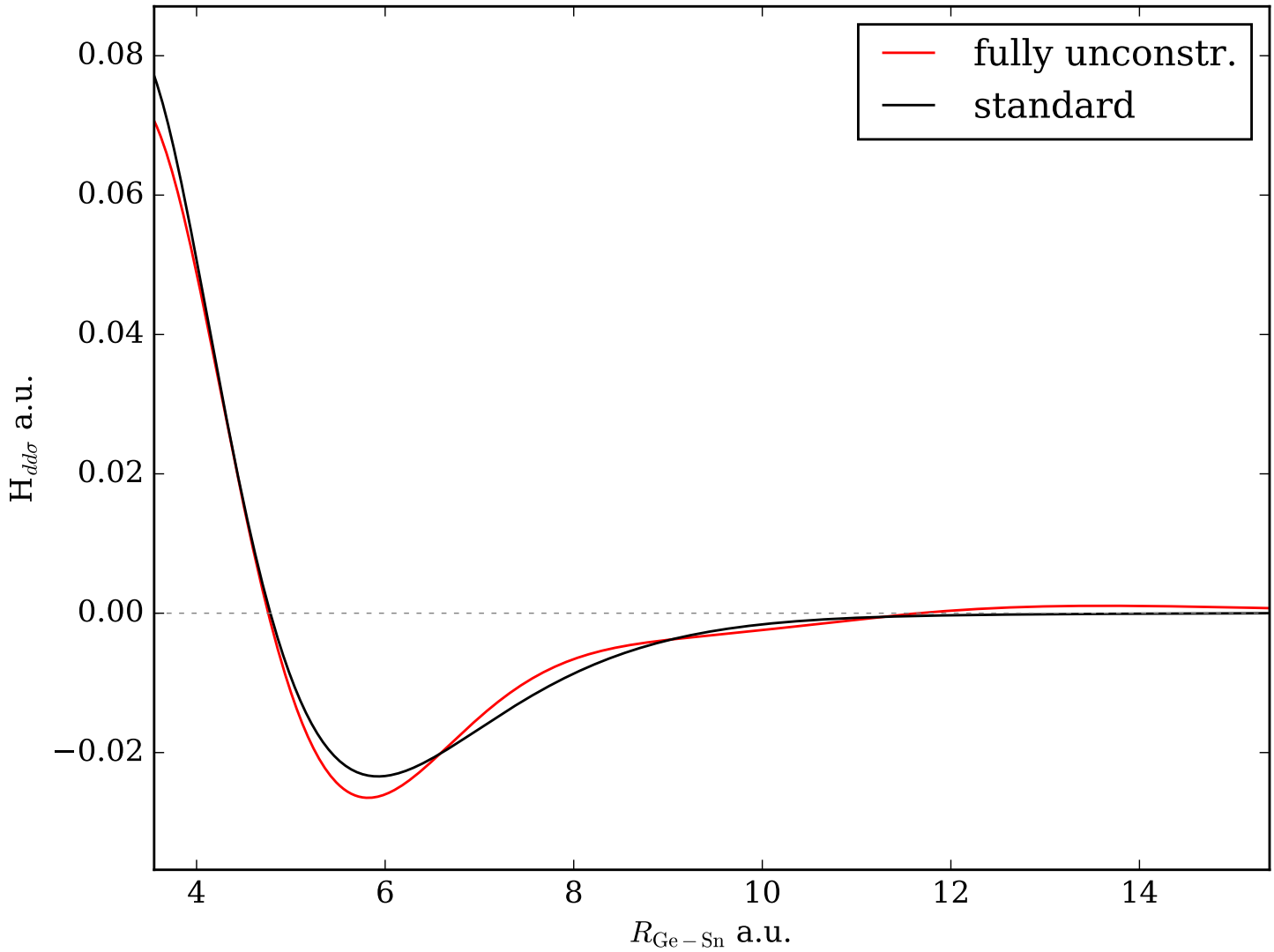

fully unconstr.
standard
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
$S_{sd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.

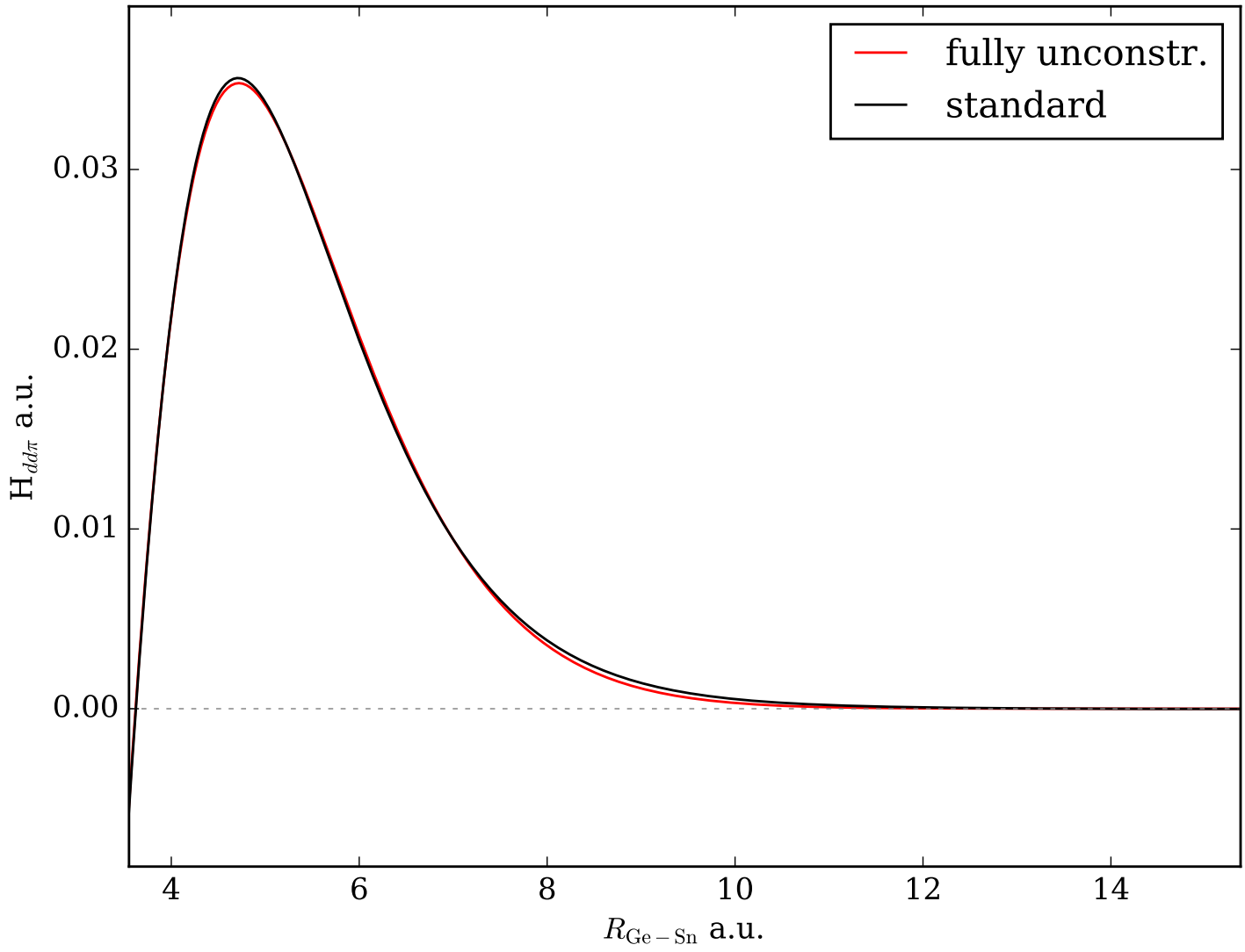

0.0
−0.1
−0.2
−0.3
−0.4
$S_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.
fully unconstr.
standard

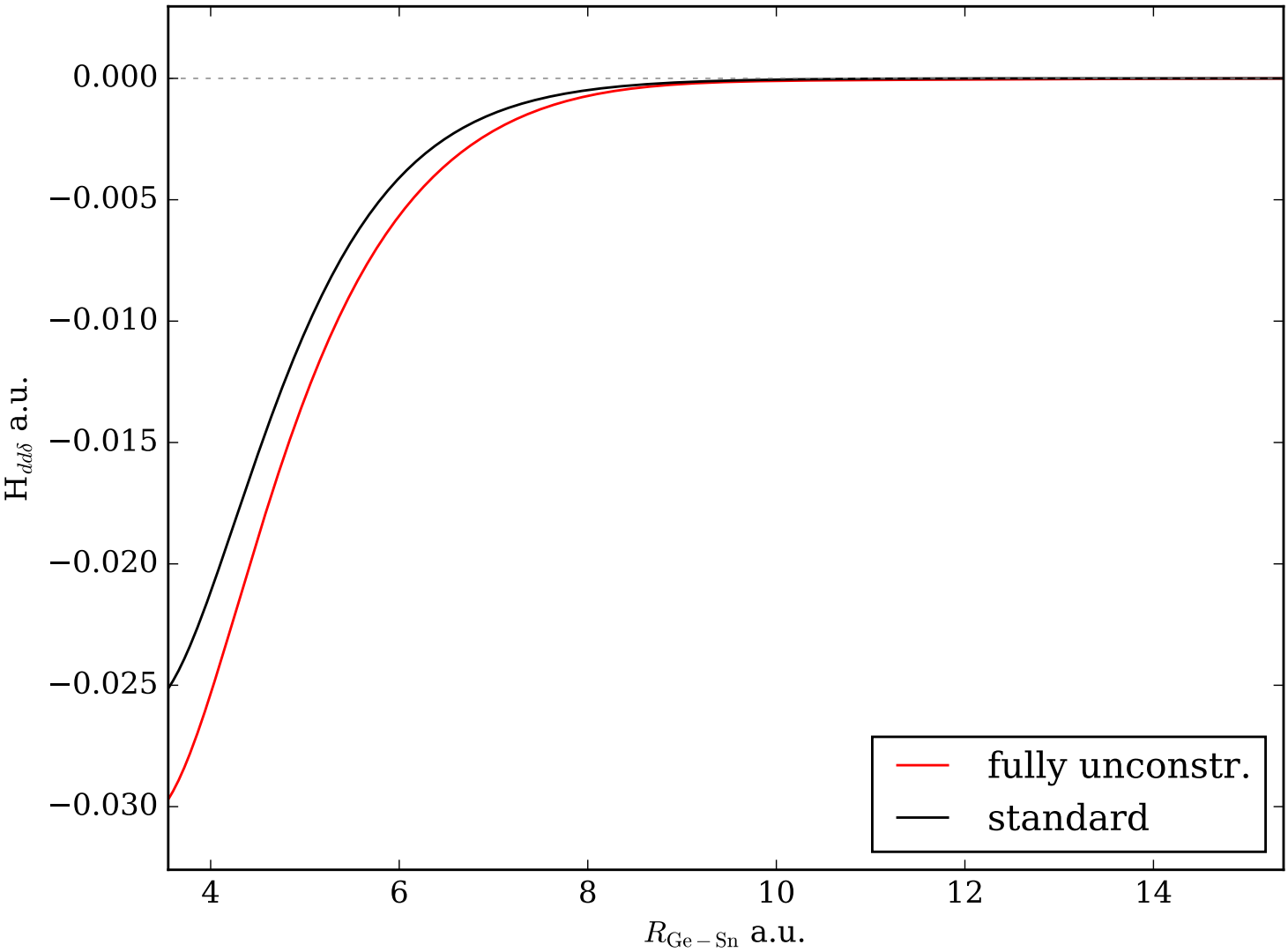

fully unconstr.
standard
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$S_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Si}}$ a.u.

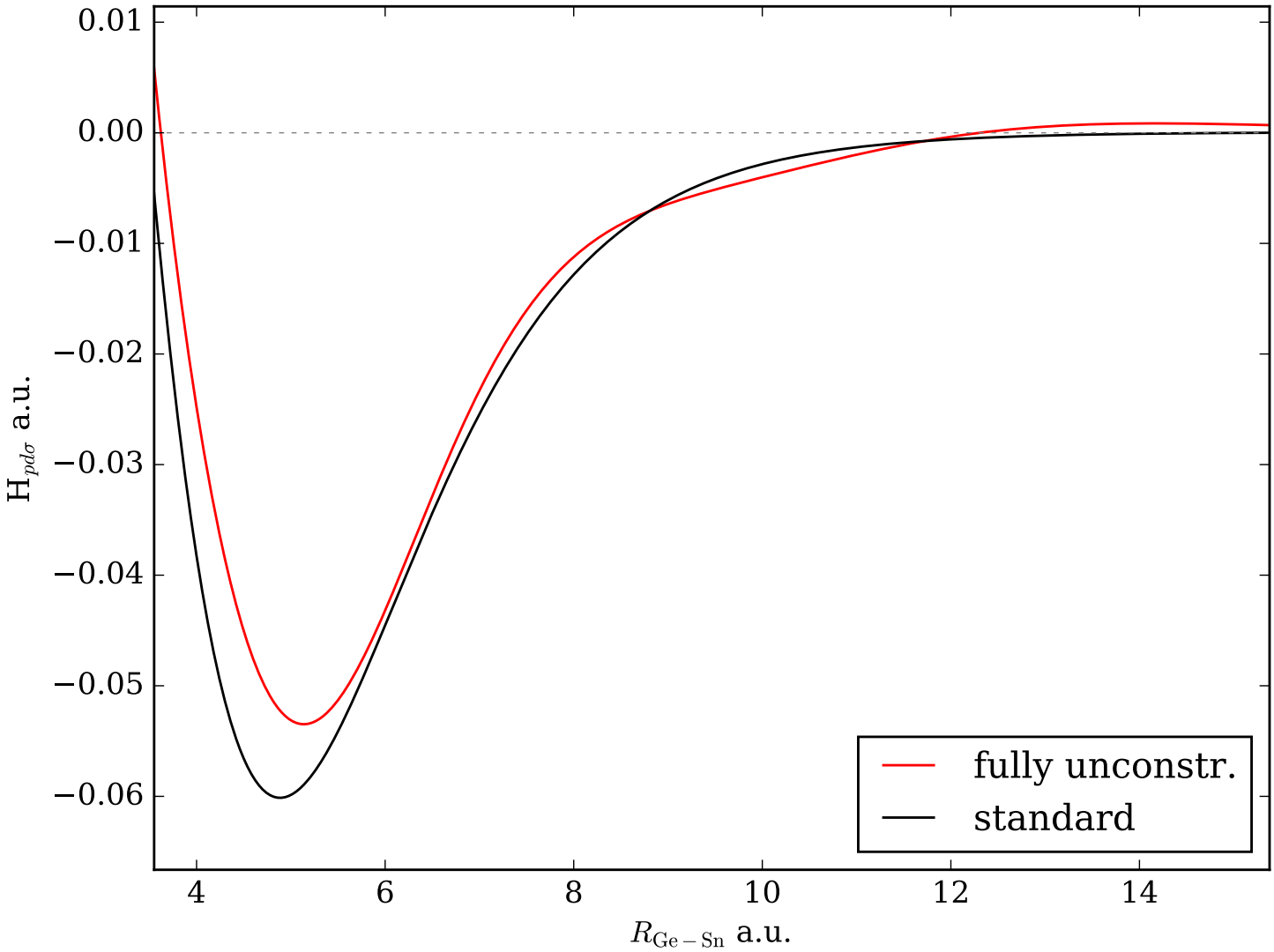
15 Ge-Sn

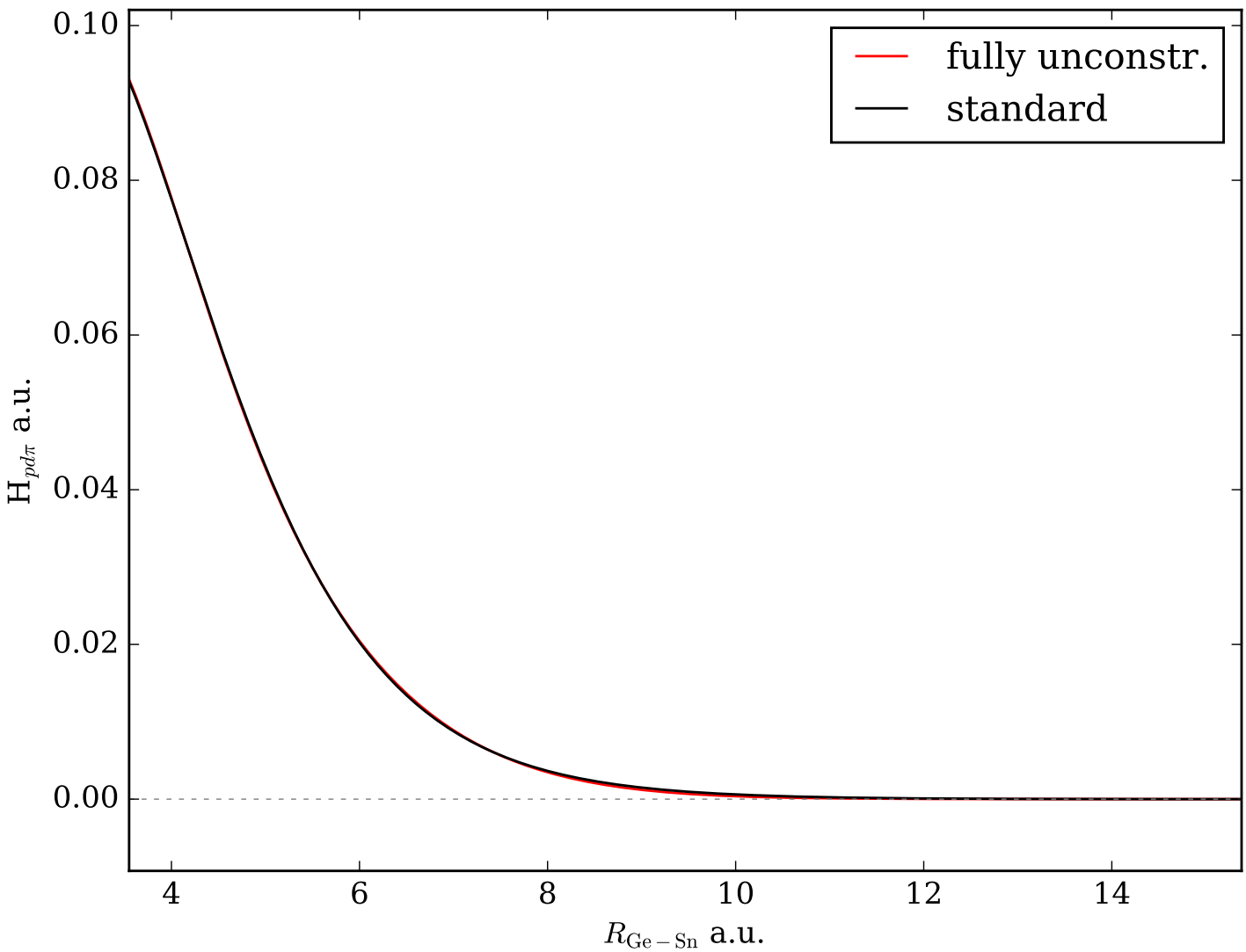
15.1 Electronic

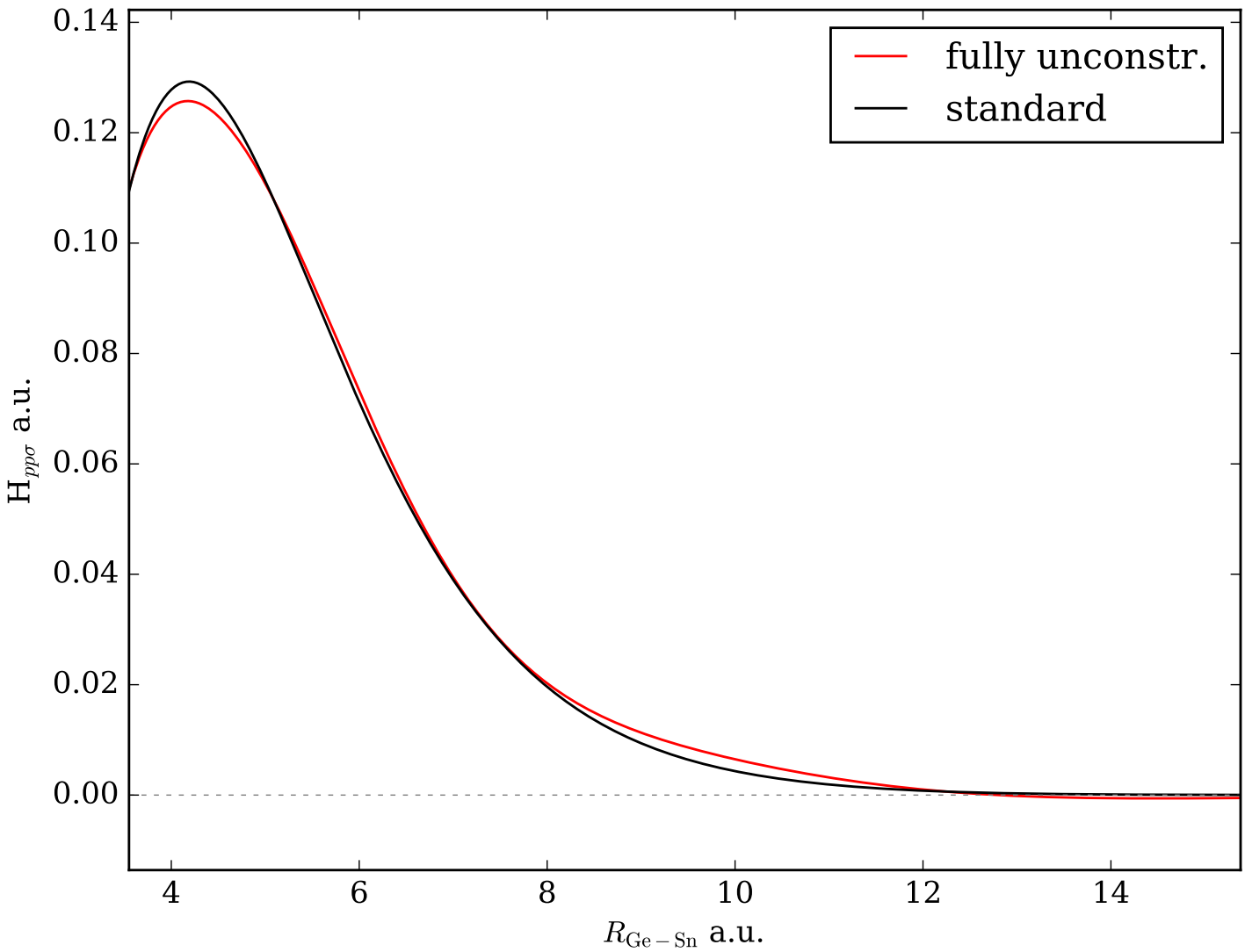


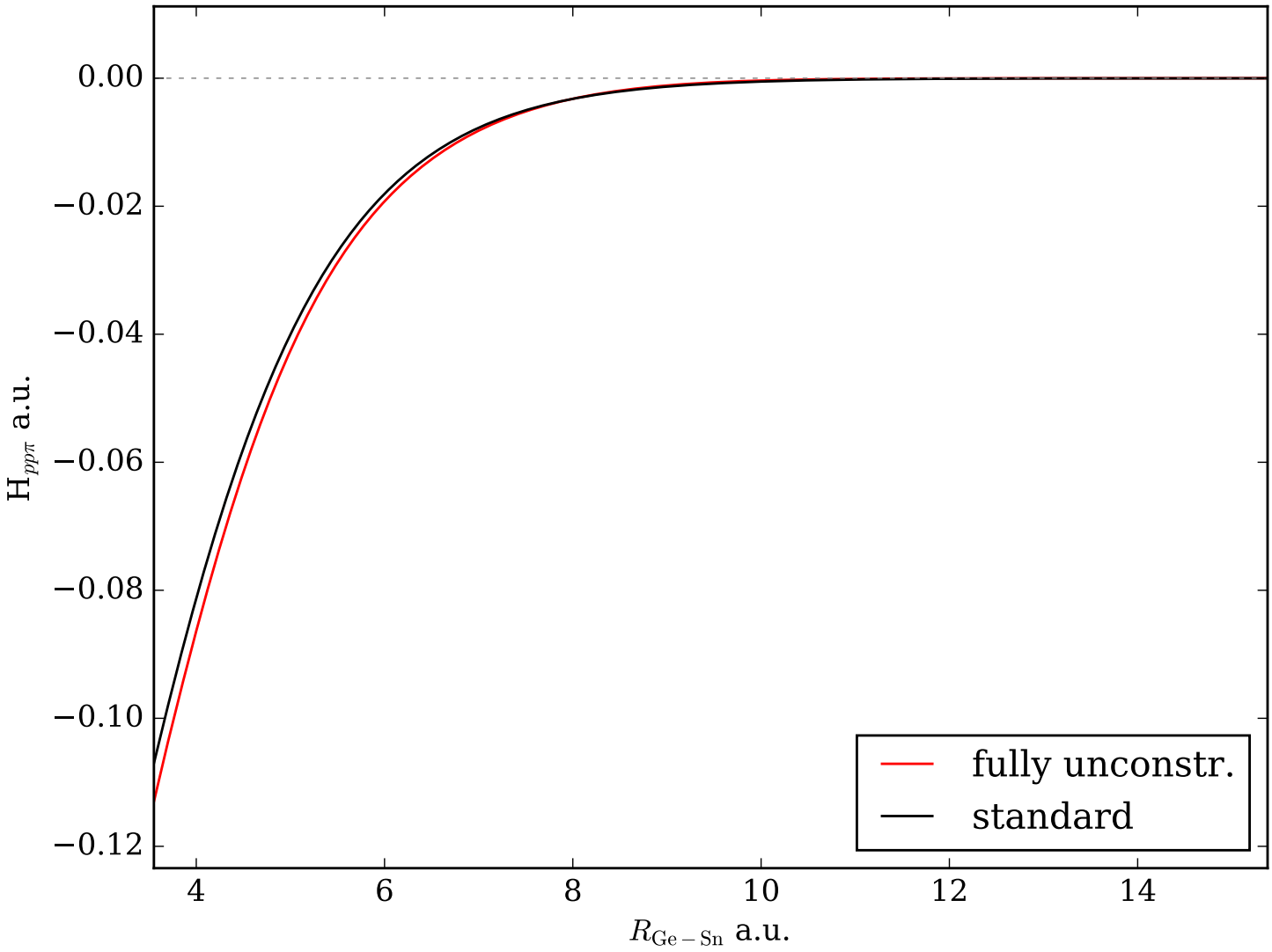

fully unconstr.
standard
0.03
0.02
0.01
0.00
$H_{dd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.

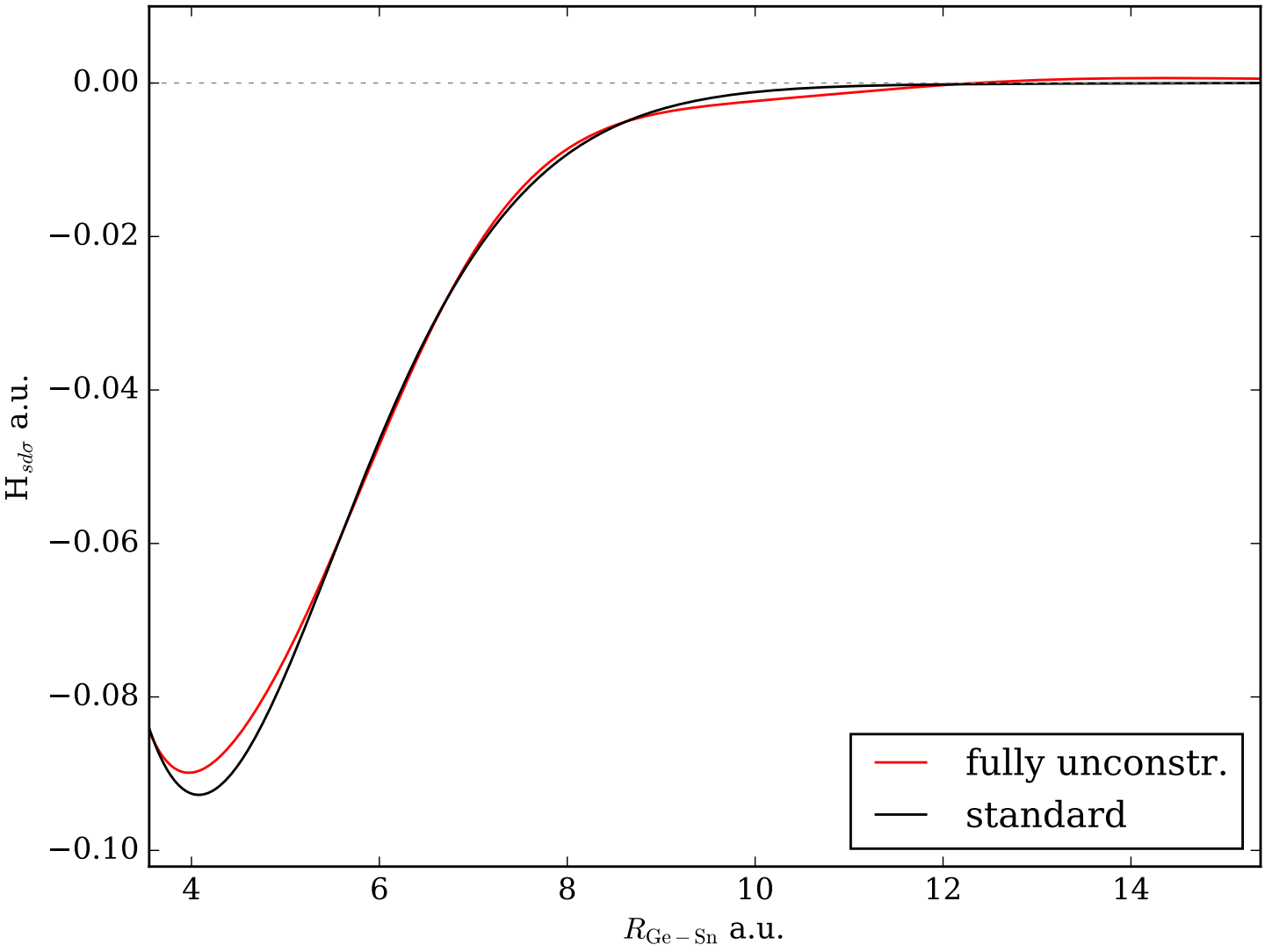

0.000
−0.005
−0.010
−0.015
−0.020
−0.025
−0.030
$H_{dd\delta}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.
fully unconstr.
standard

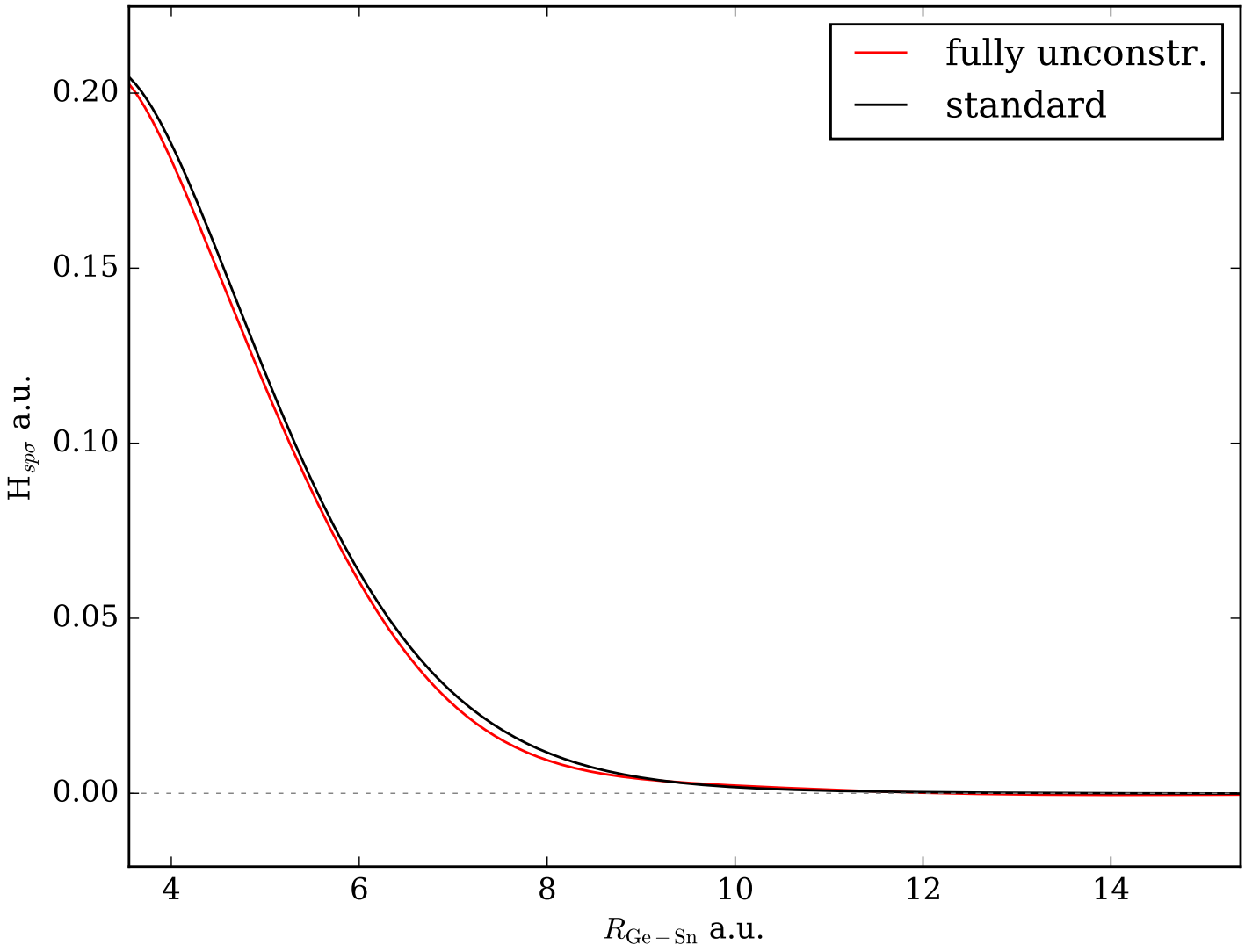

0.01
0.00
−0.01
−0.02
−0.03
−0.04
−0.05
−0.06
$H_{pd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.
fully unconstr.
standard

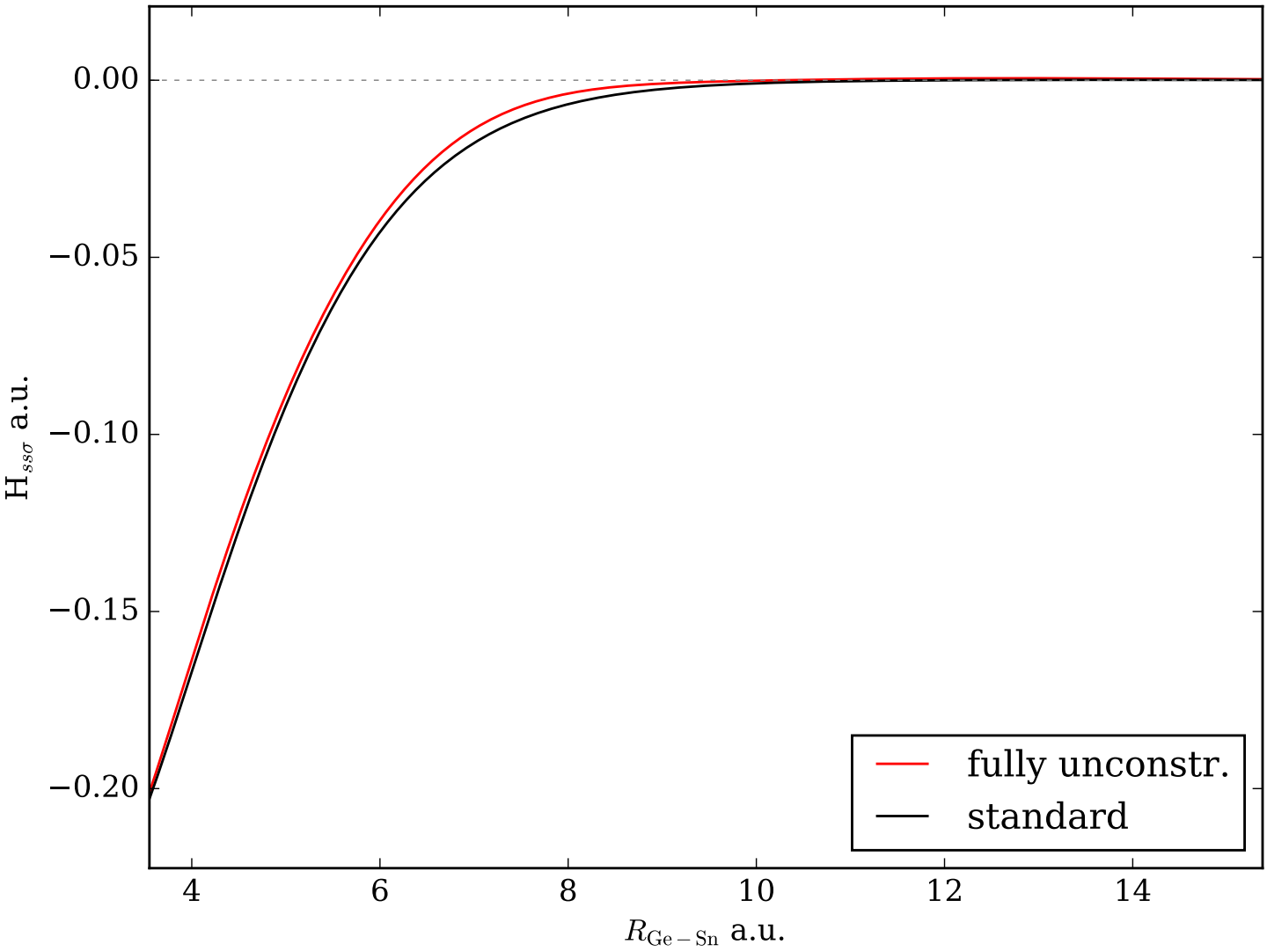

fully unconstr.
standard
0.10
0.08
0.06
0.04
0.02
0.00
$H_{pd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.

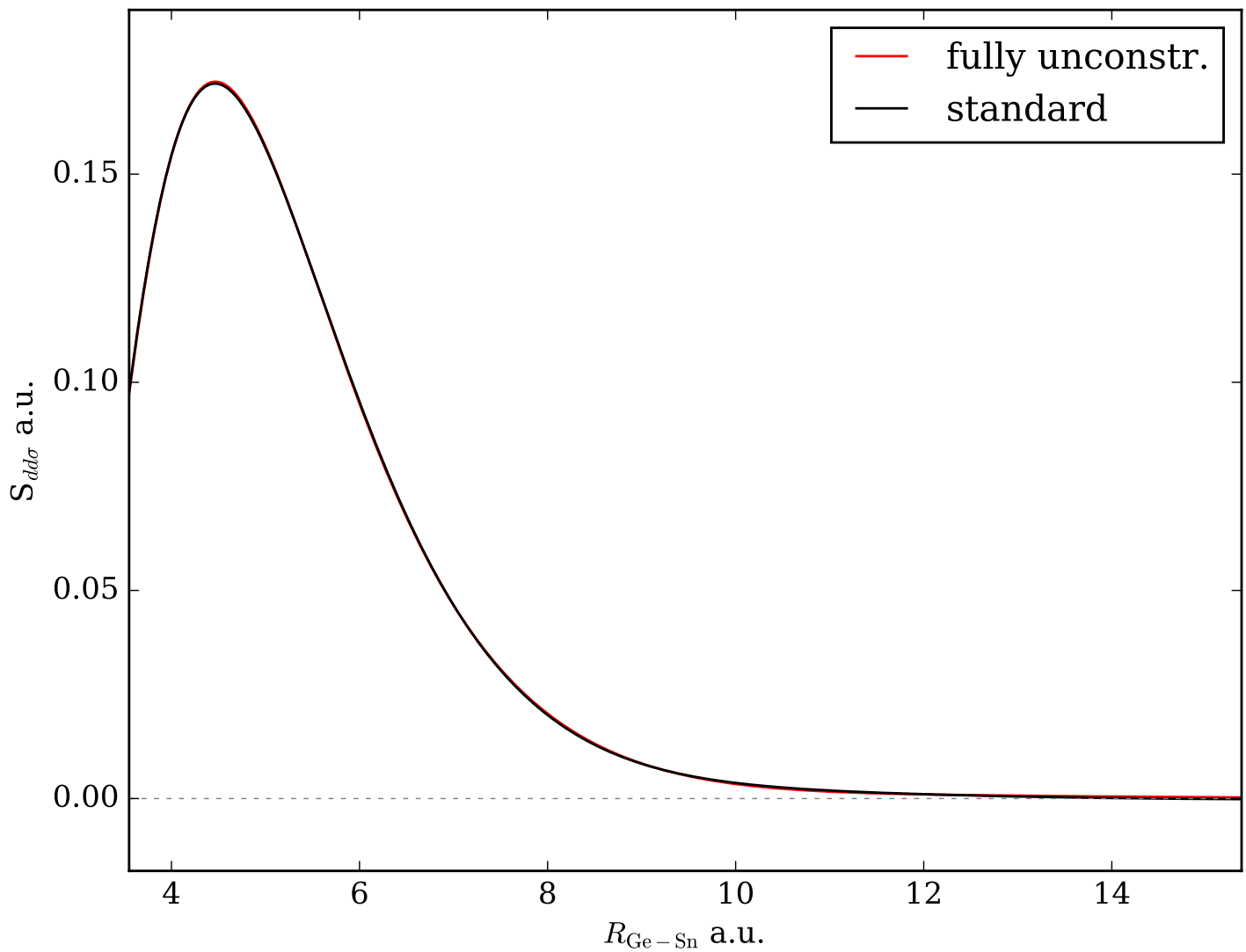

fully unconstr.
standard
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
$H_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.

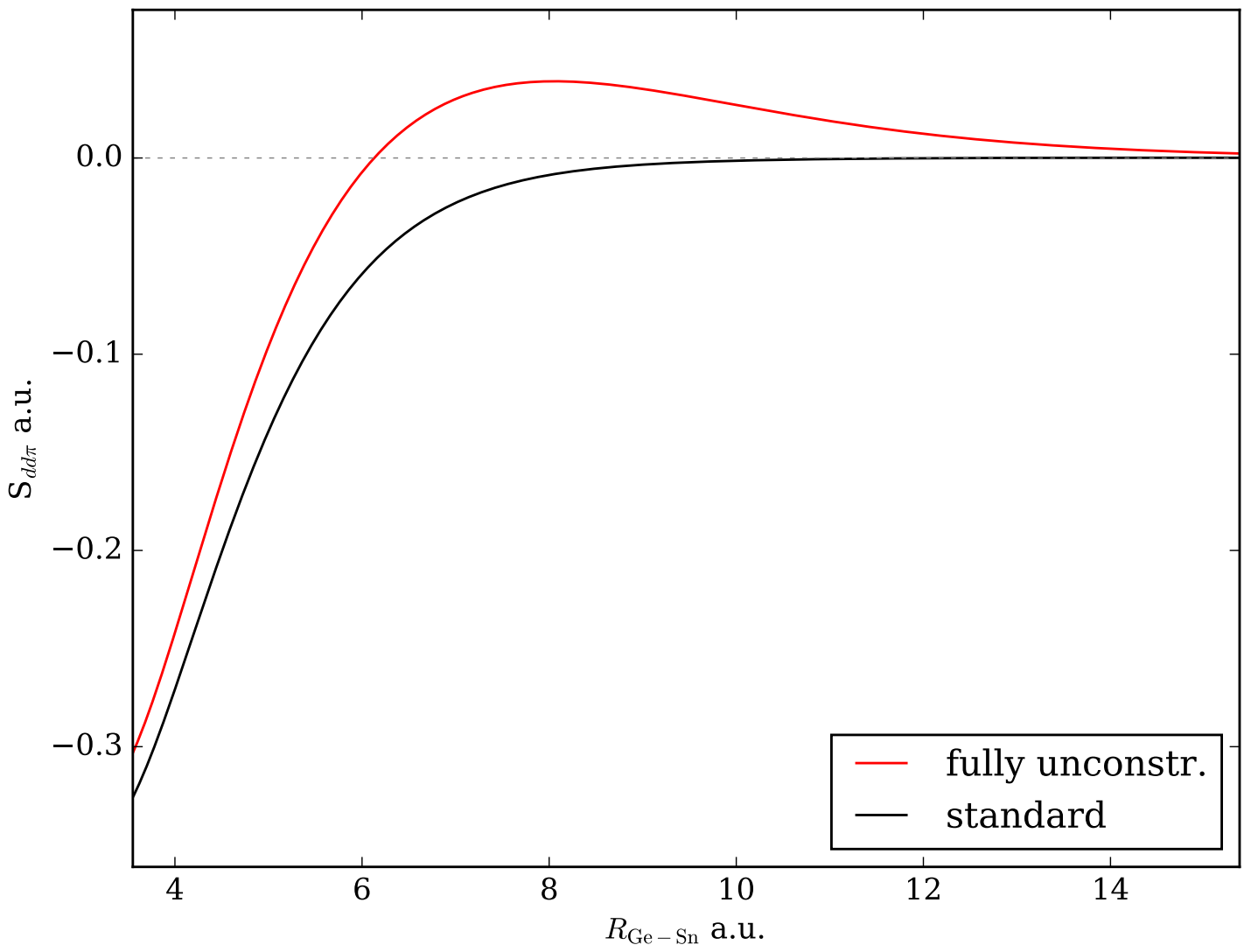

0.00
−0.02
−0.04
−0.06
−0.08
−0.10
−0.12
$H_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.
fully unconstr.
standard

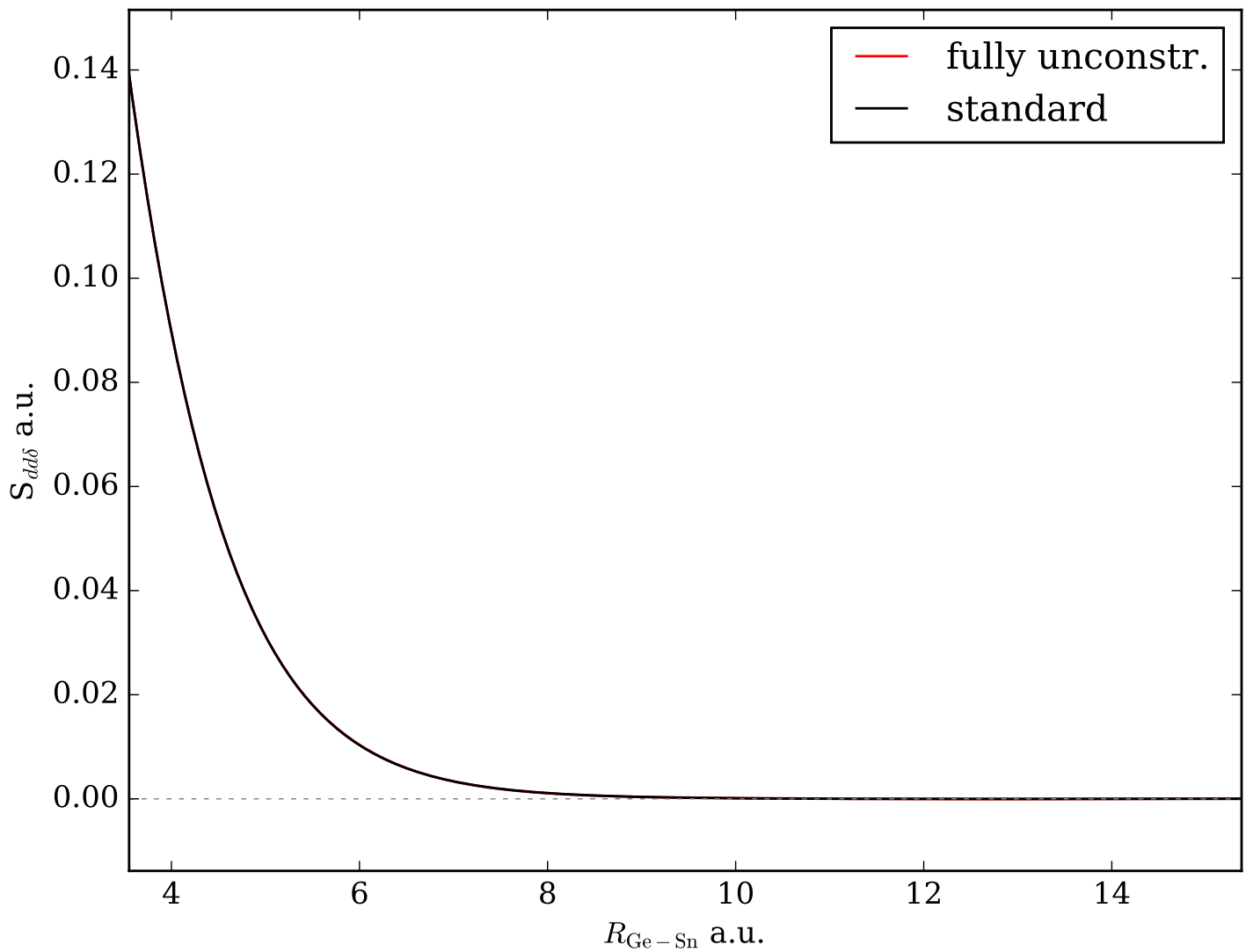

0.00
−0.02
−0.04
−0.06
−0.08
−0.10
$H_{sd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.
fully unconstr.
standard

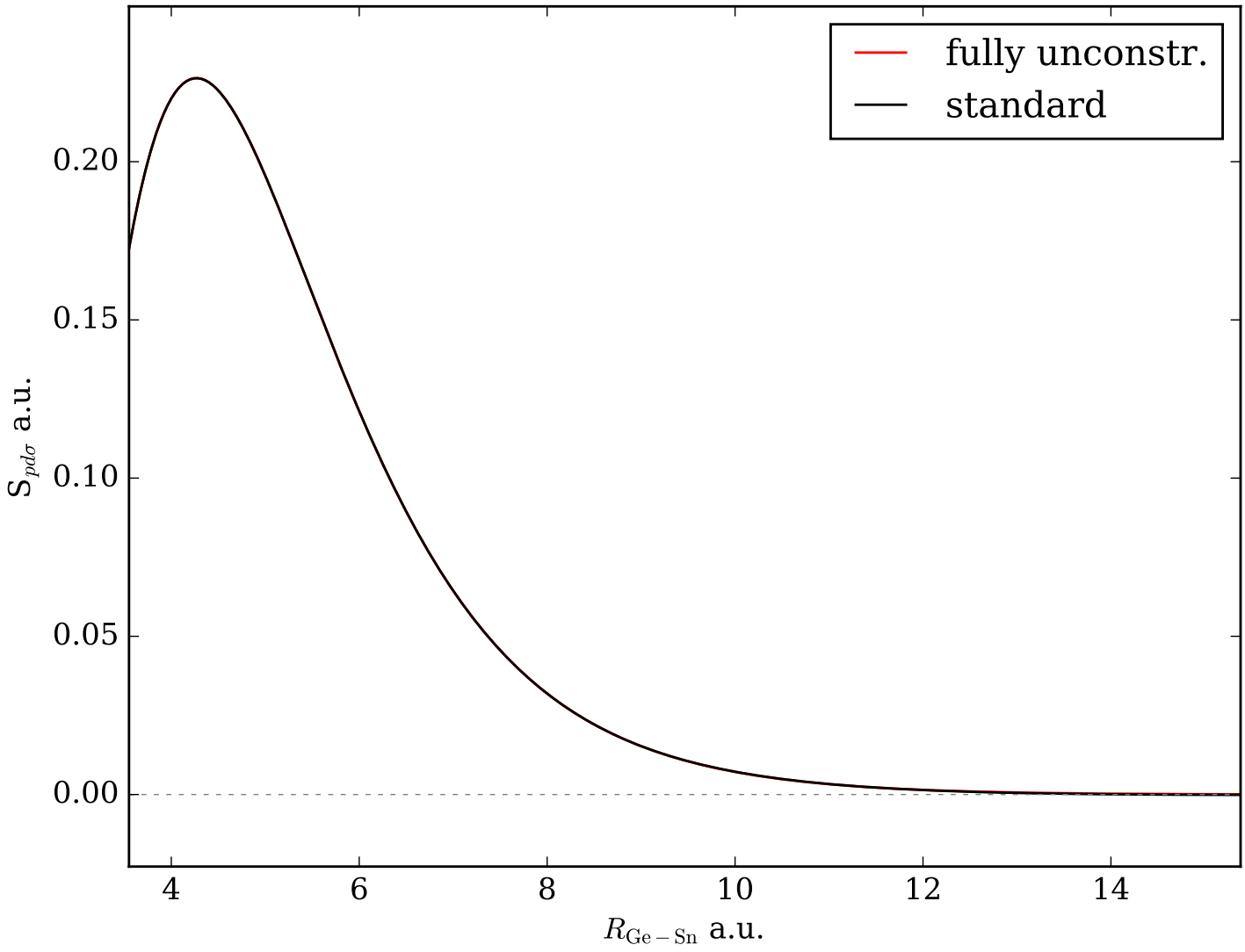

fully unconstr.
standard
0.20
0.15
0.10
0.05
0.00
$H_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.

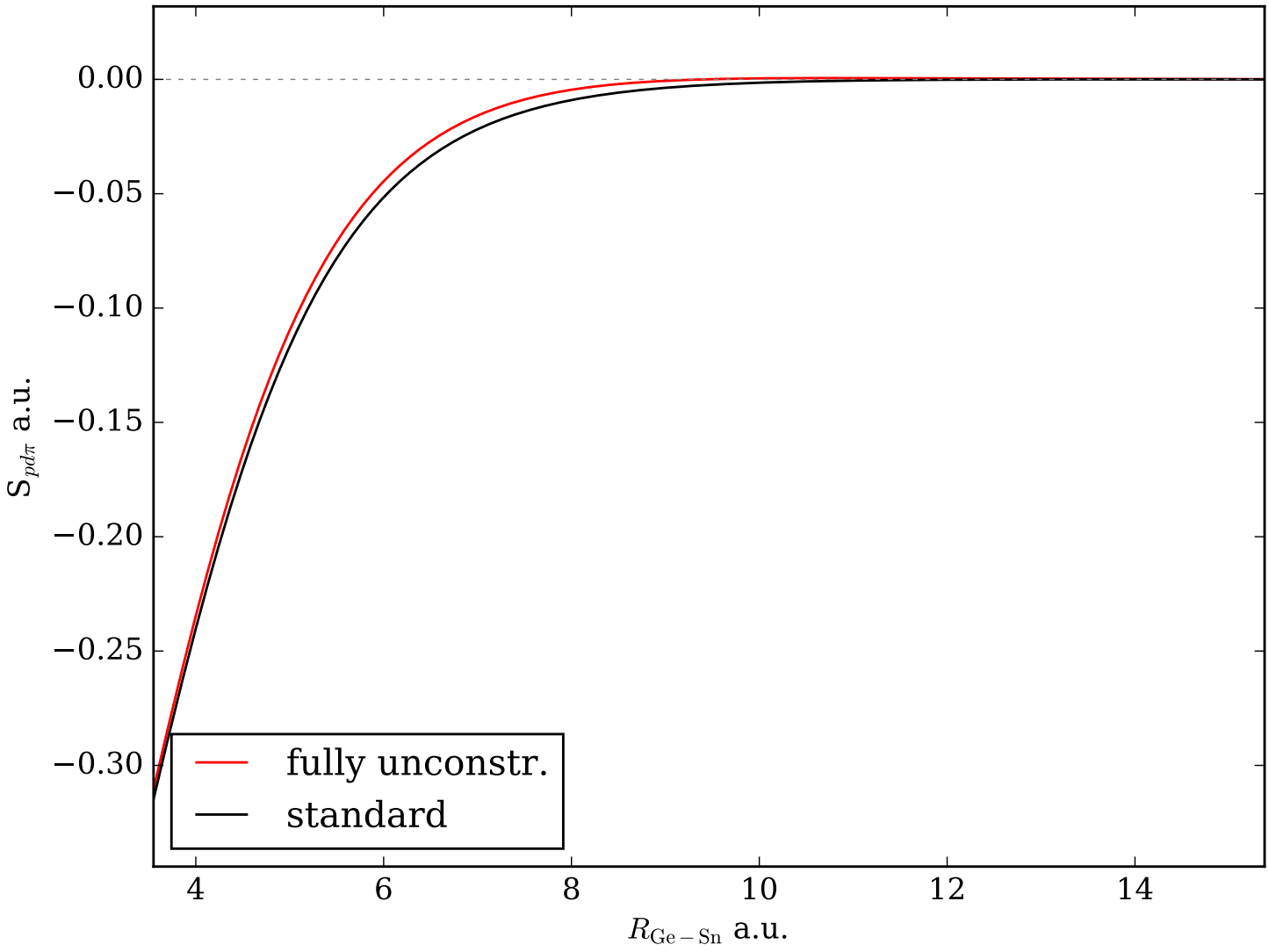

0.00
−0.05
−0.10
−0.15
−0.20
$H_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.
fully unconstr.
standard

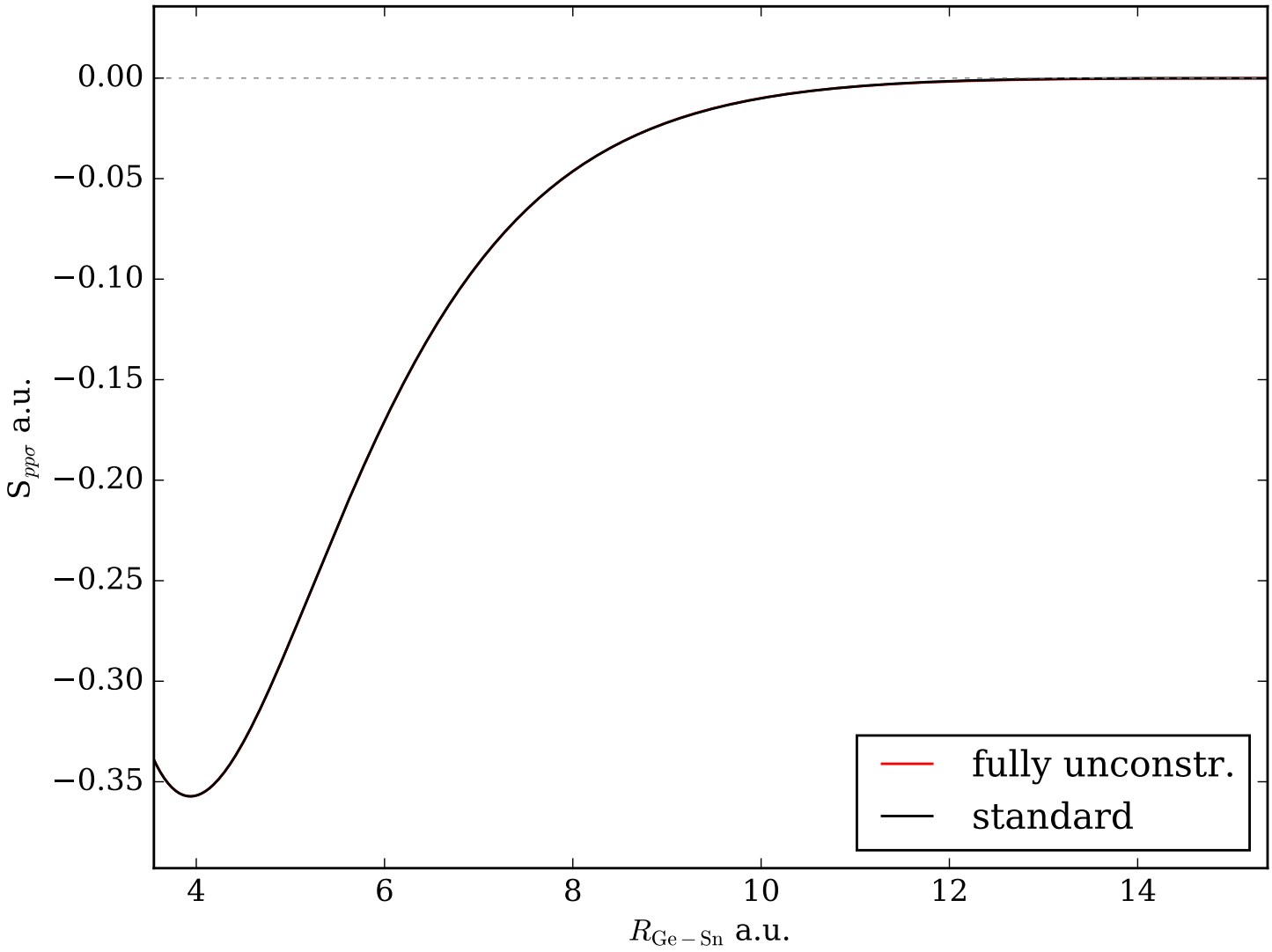

fully unconstr.
standard
0.15
0.10
0.05
0.00
$S_{dd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.

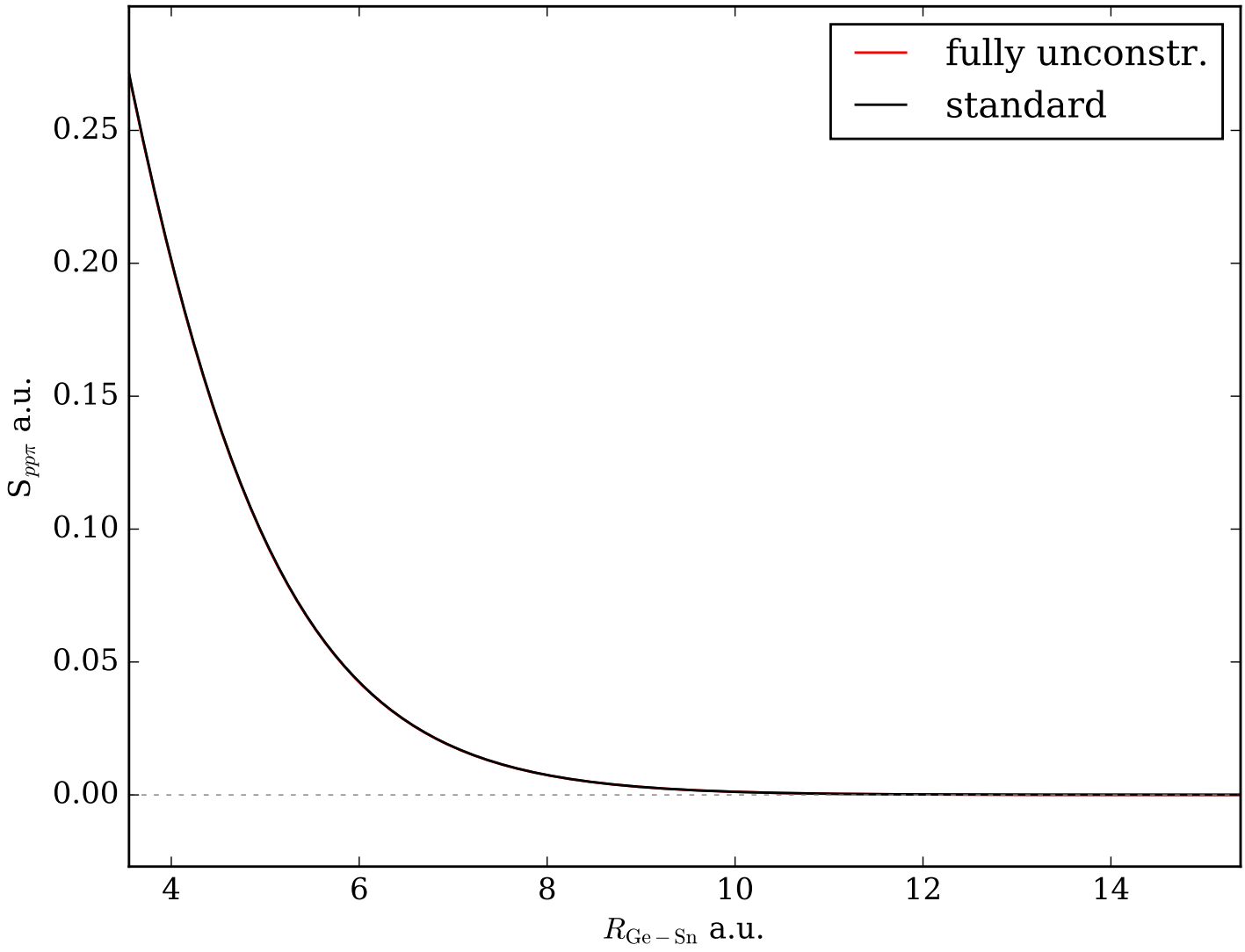

0.0
−0.1
−0.2
−0.3
$S_{dd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.
fully unconstr.
standard

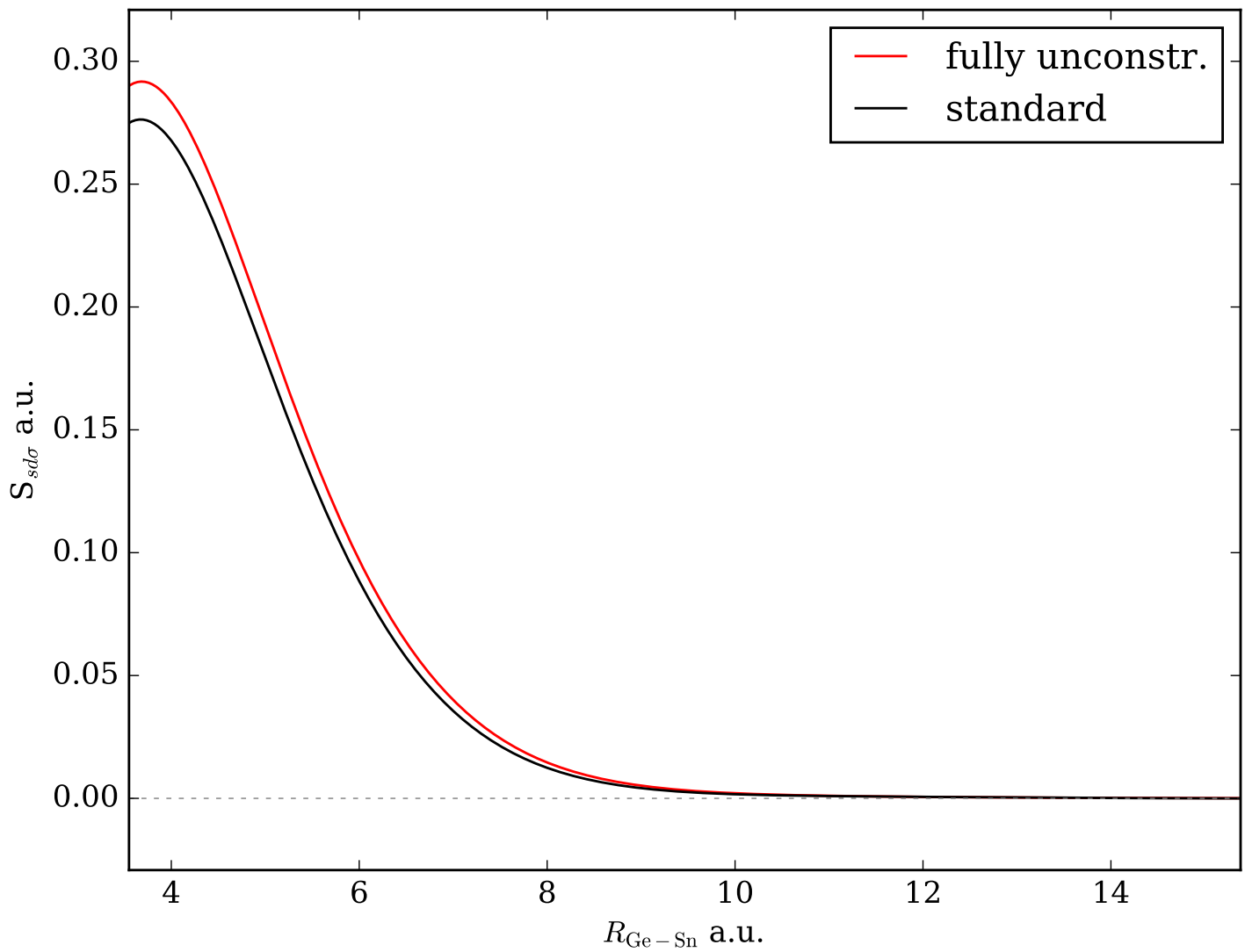

fully unconstr.
standard
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
$S_{dd\delta}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.

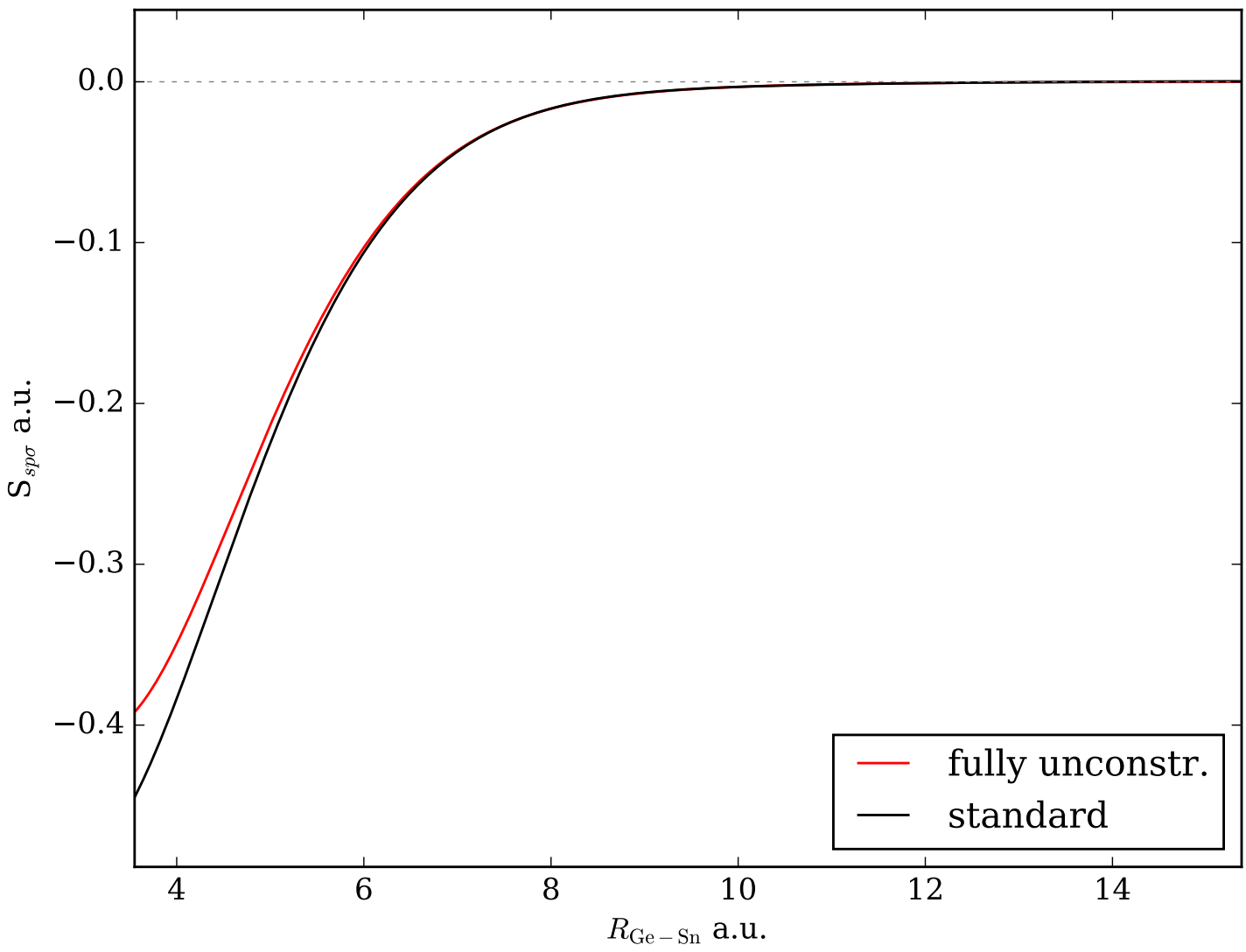

fully unconstr.
standard
0.20
0.15
0.10
0.05
0.00
$S_{pd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.

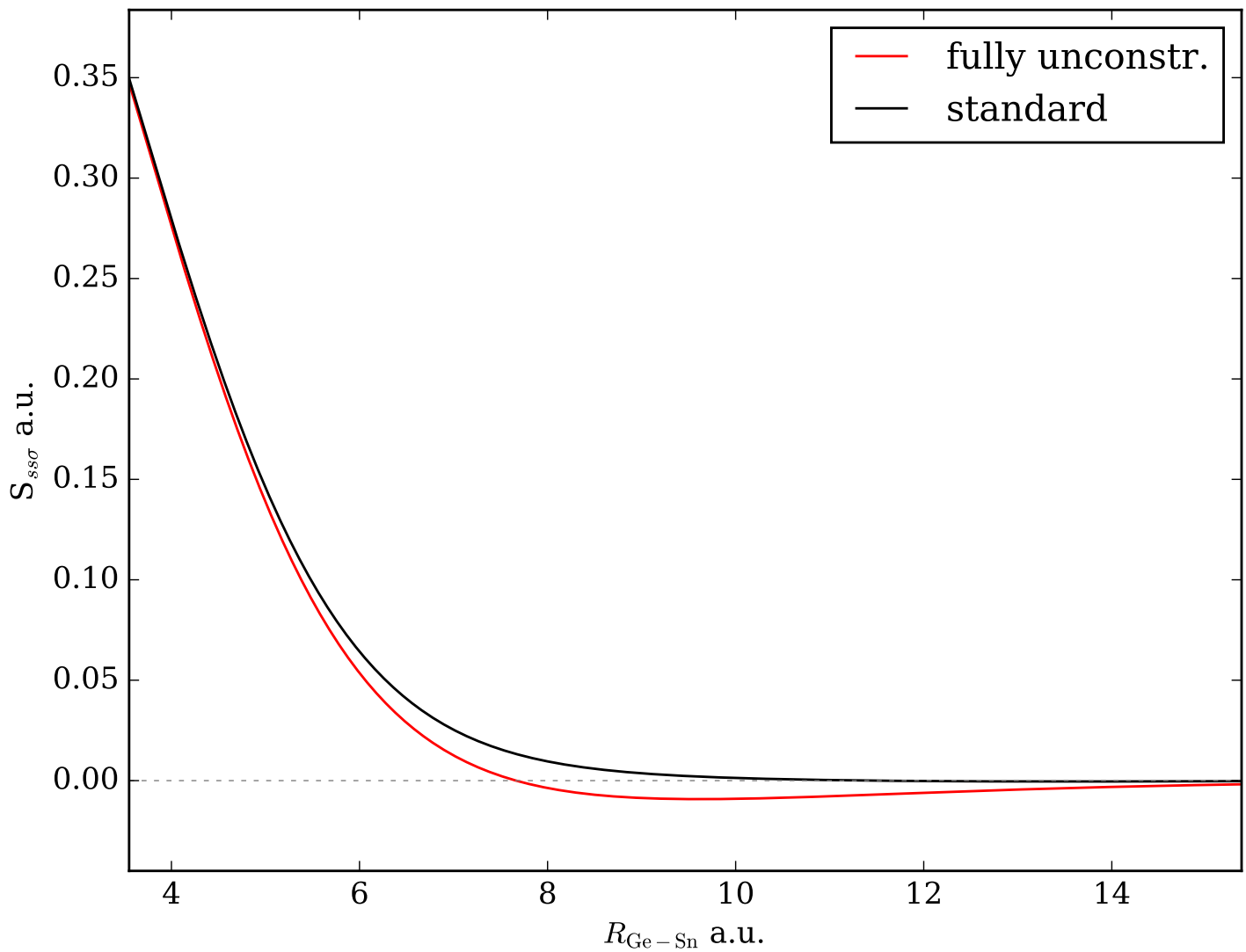

0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
$S_{pd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.
fully unconstr.
standard


0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
−0.35
$S_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.
fully unconstr.
standard

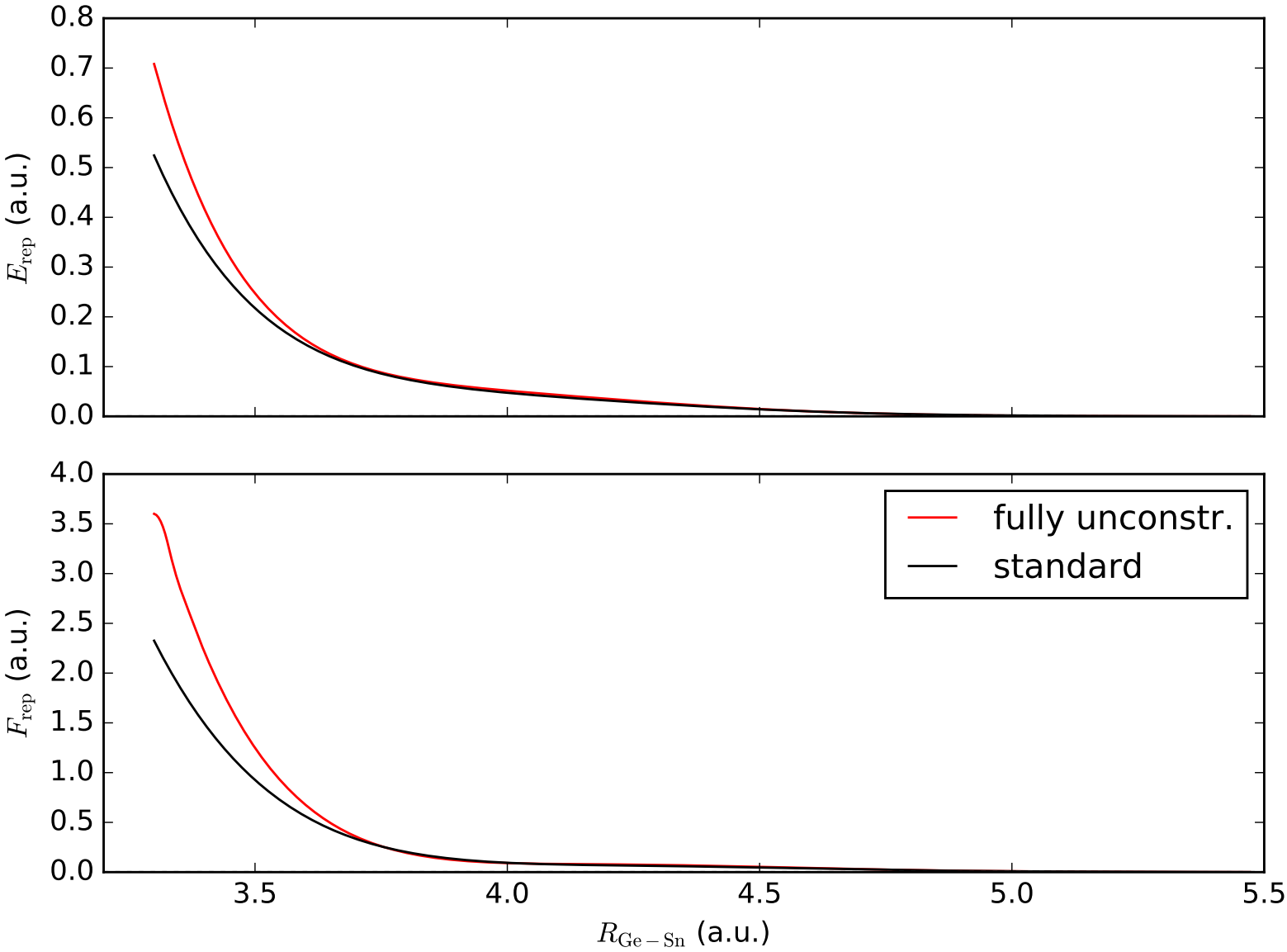

fully unconstr.
standard
0.25
0.20
0.15
0.10
0.05
0.00
$S_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.


fully unconstr.
standard
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$S_{sd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.


0.0
−0.1
−0.2
−0.3
−0.4
$S_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.
fully unconstr.
standard

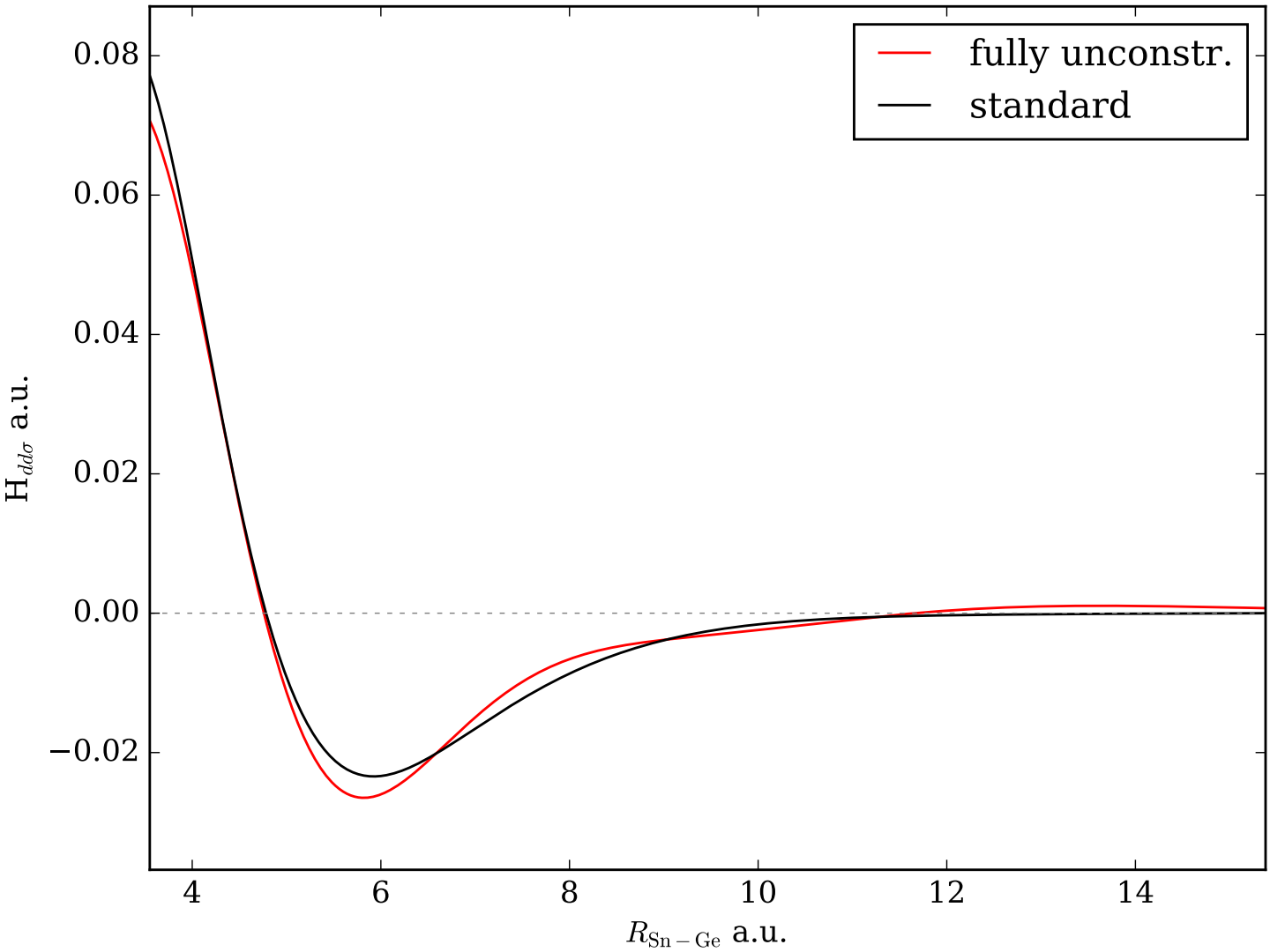

fully unconstr.
standard
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$S_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Ge-Sn}}$ a.u.

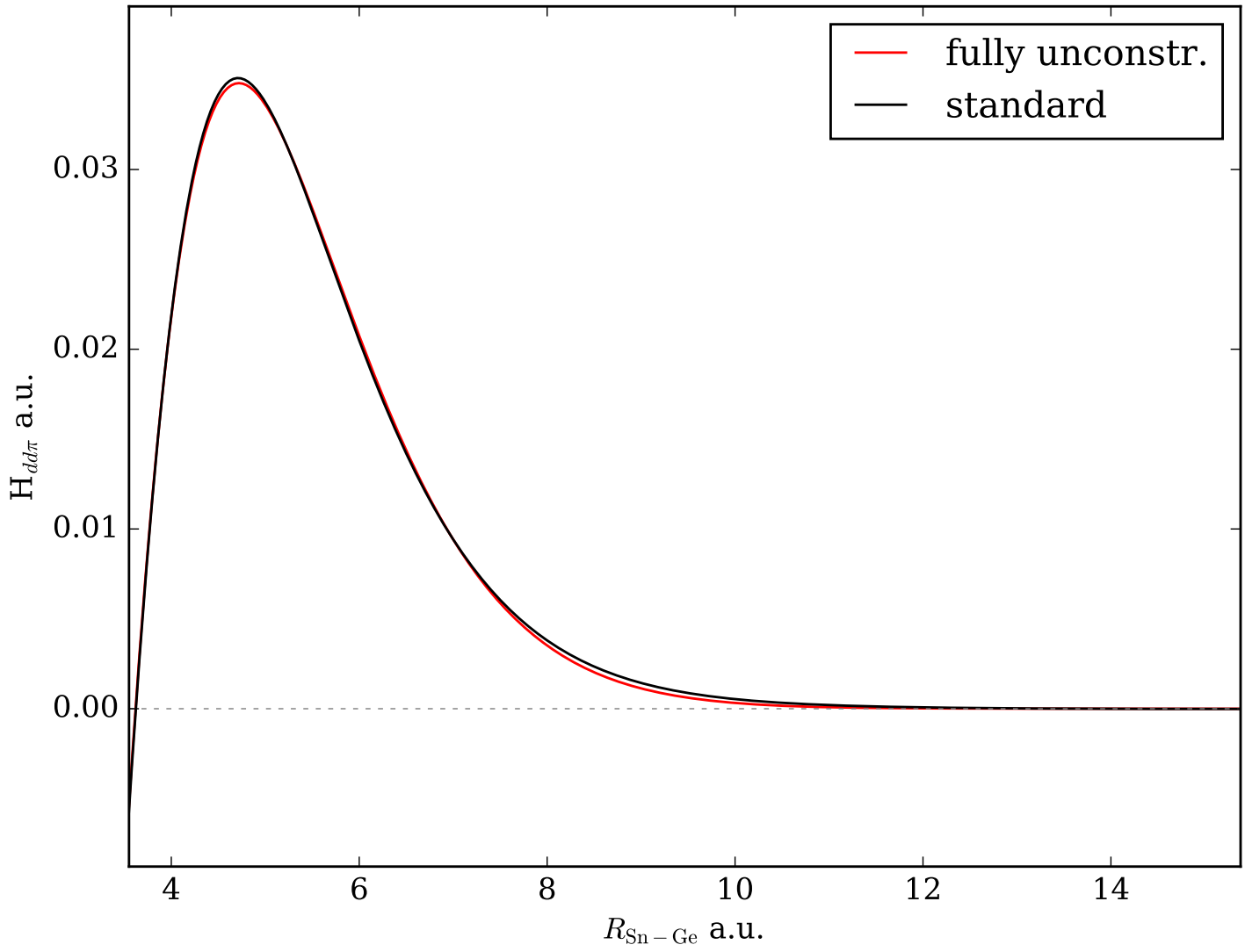
15.2 Repulsive

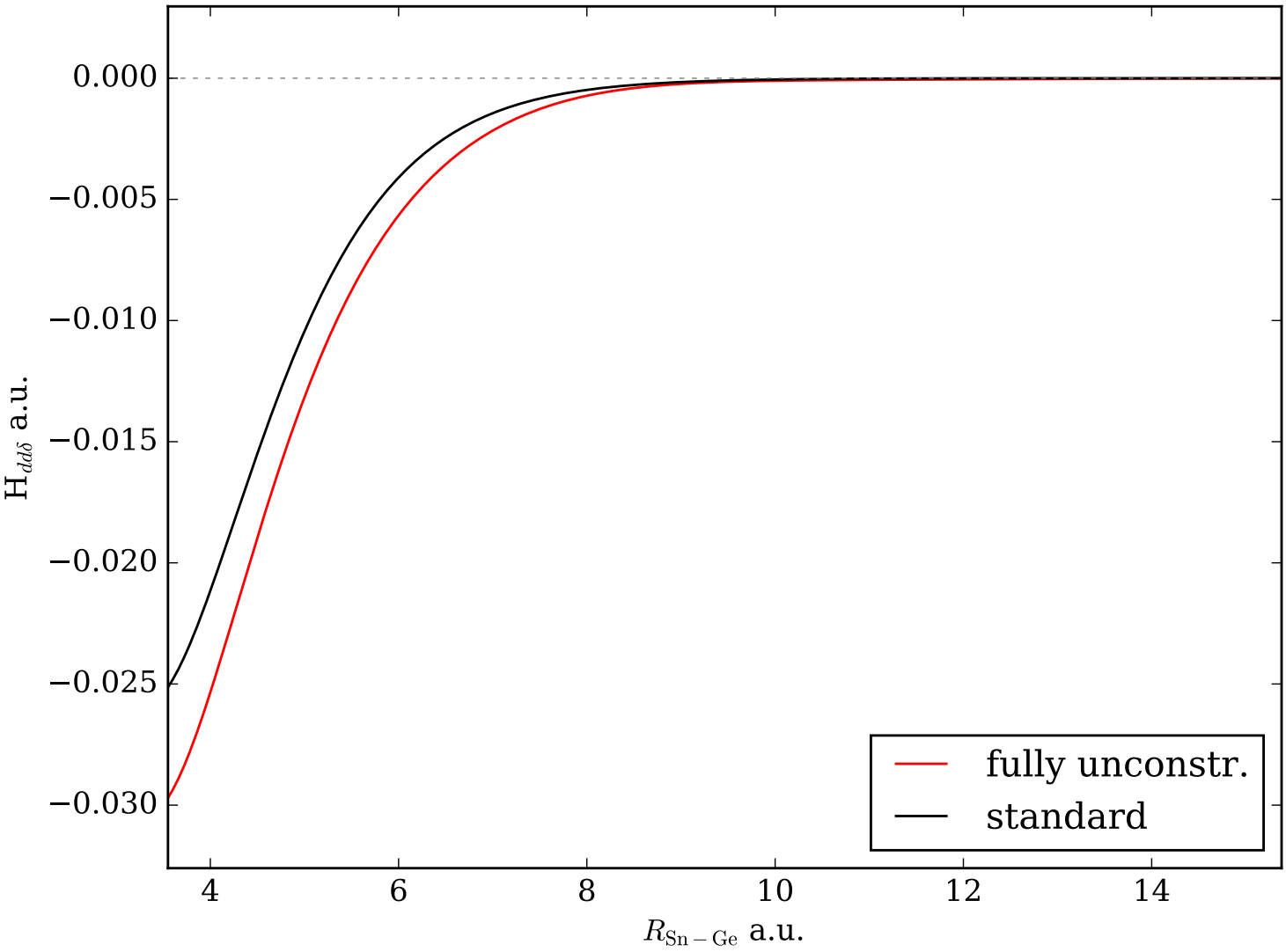


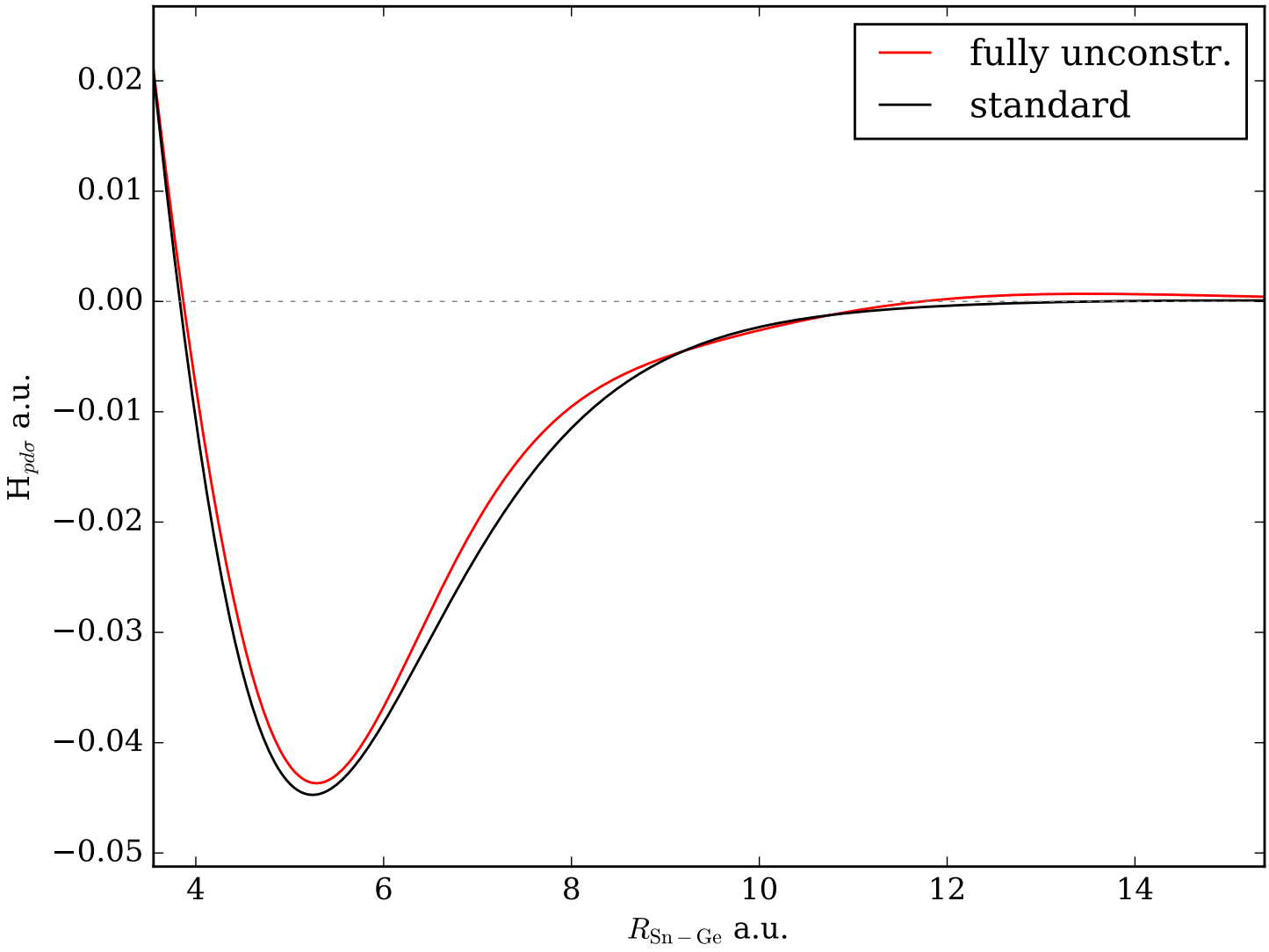
16 Sn-Ge

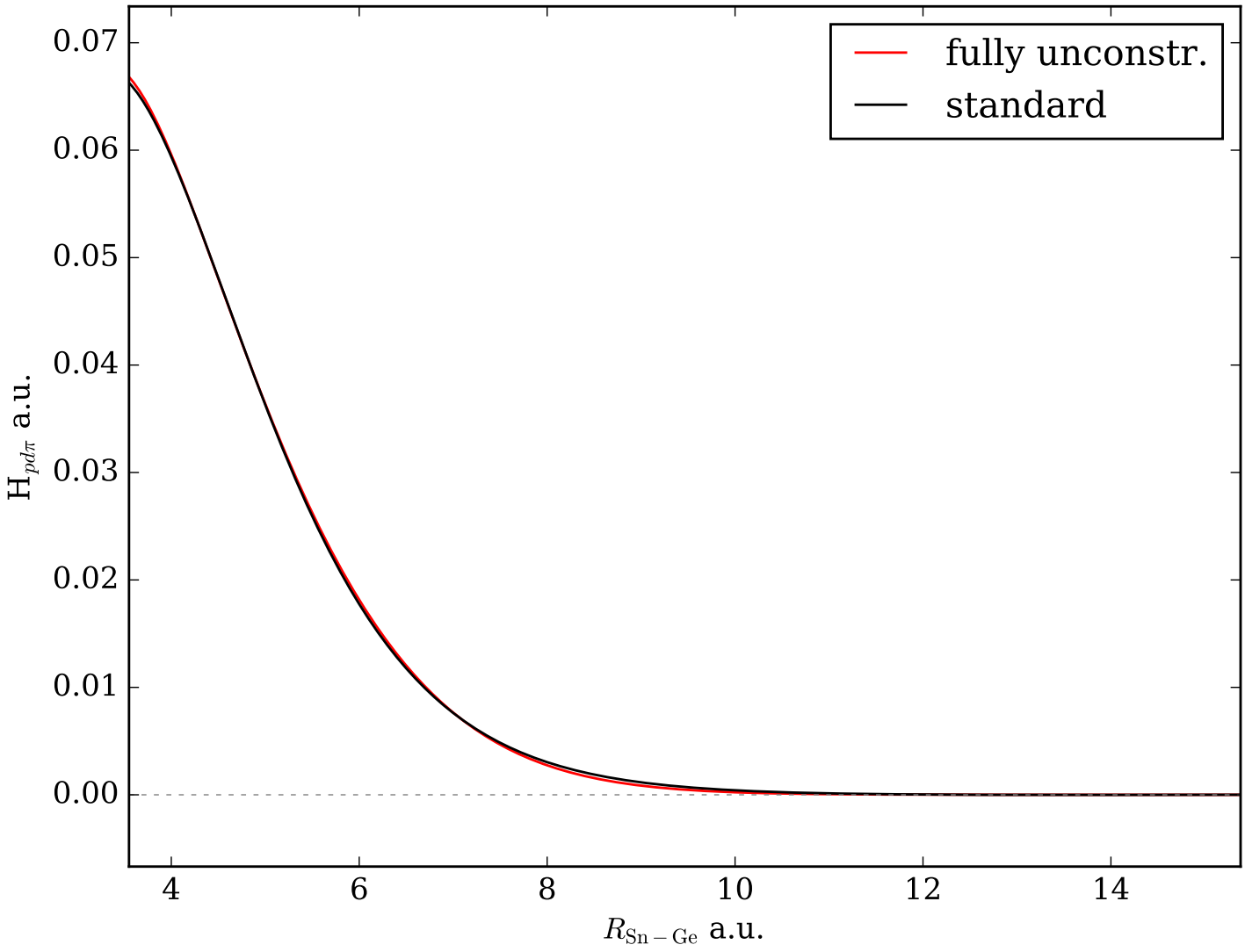
16.1 Electronic

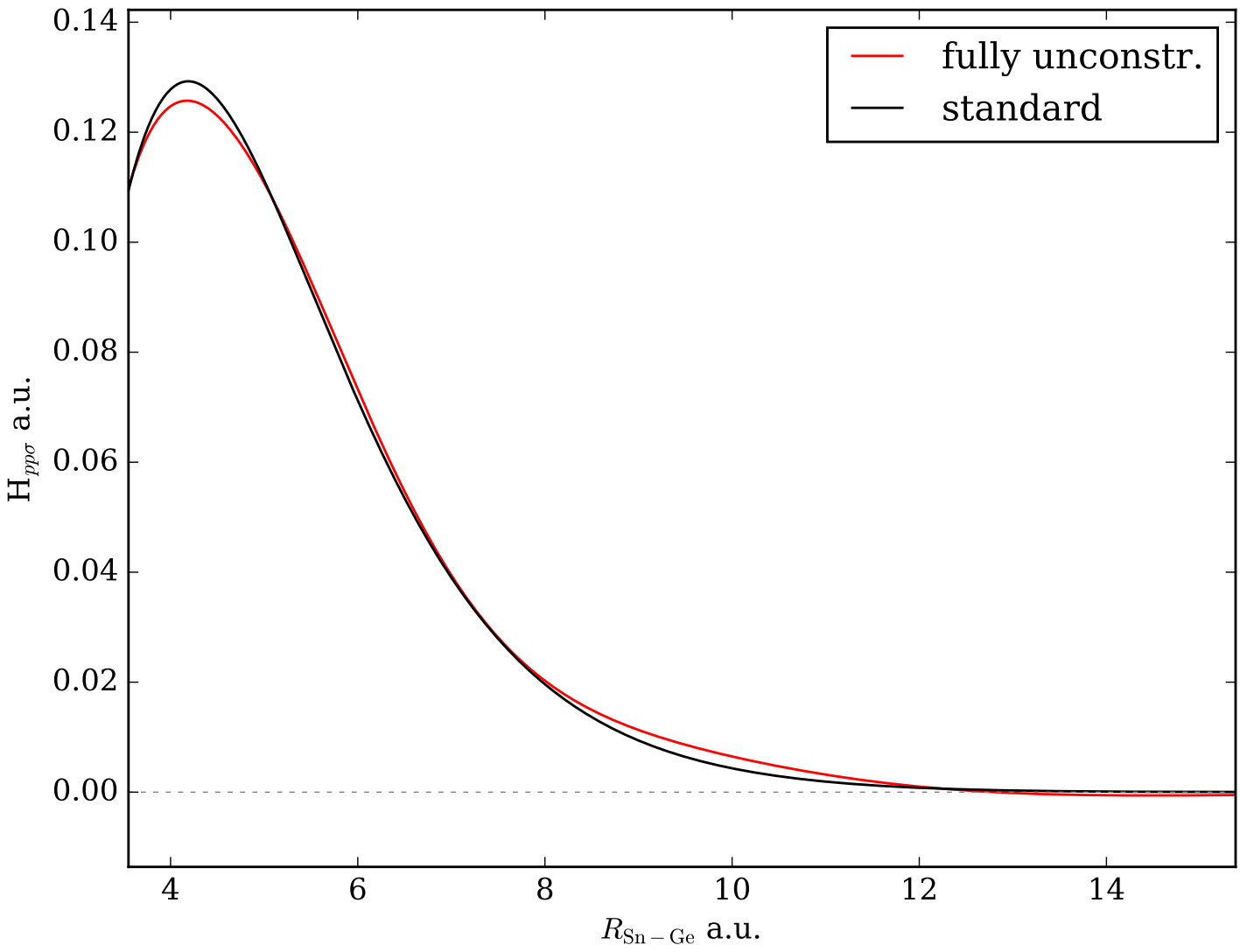


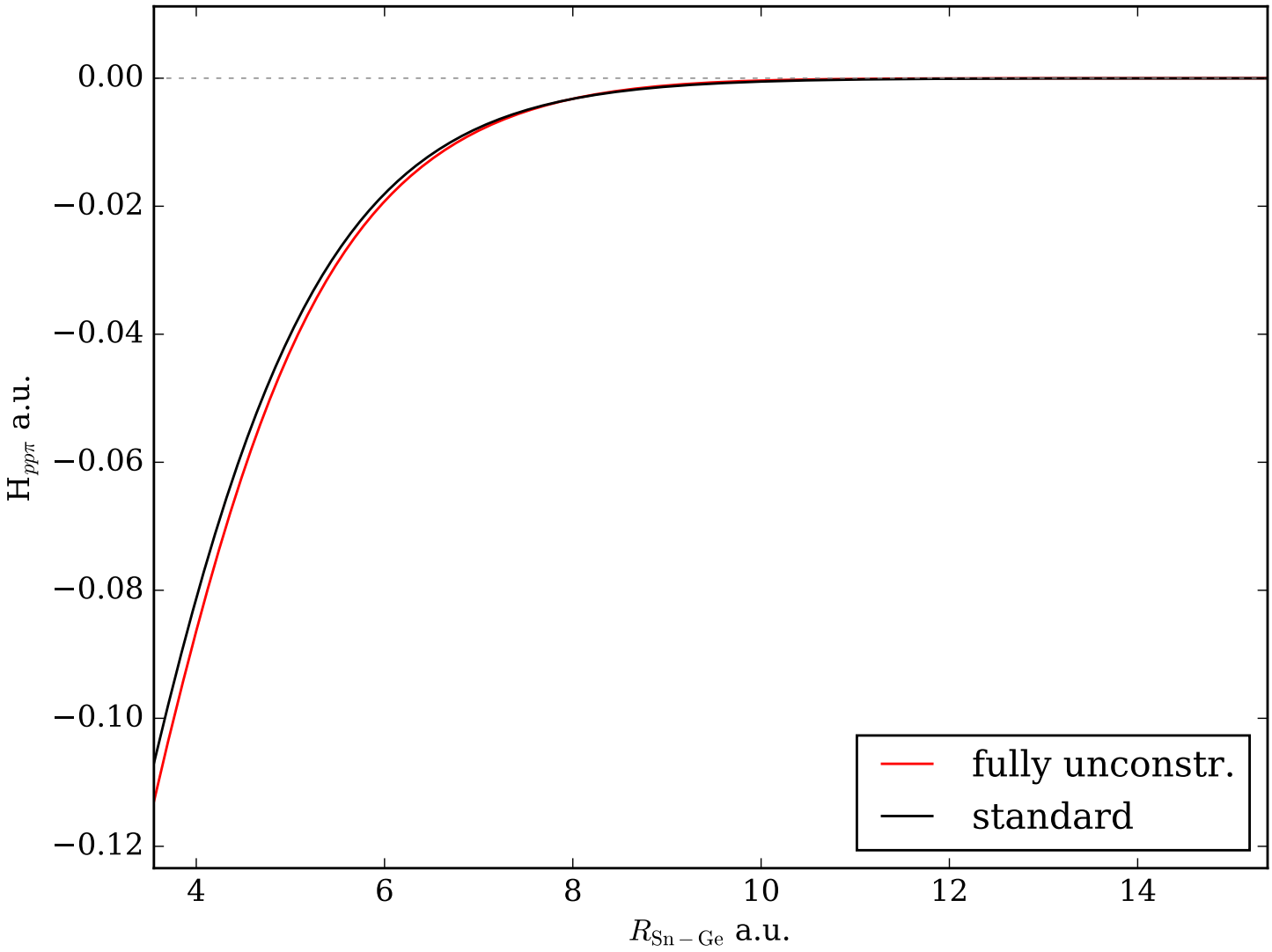

fully unconstr.
standard
0.03
0.02
0.01
0.00
$H_{dd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Ge}}$ a.u.

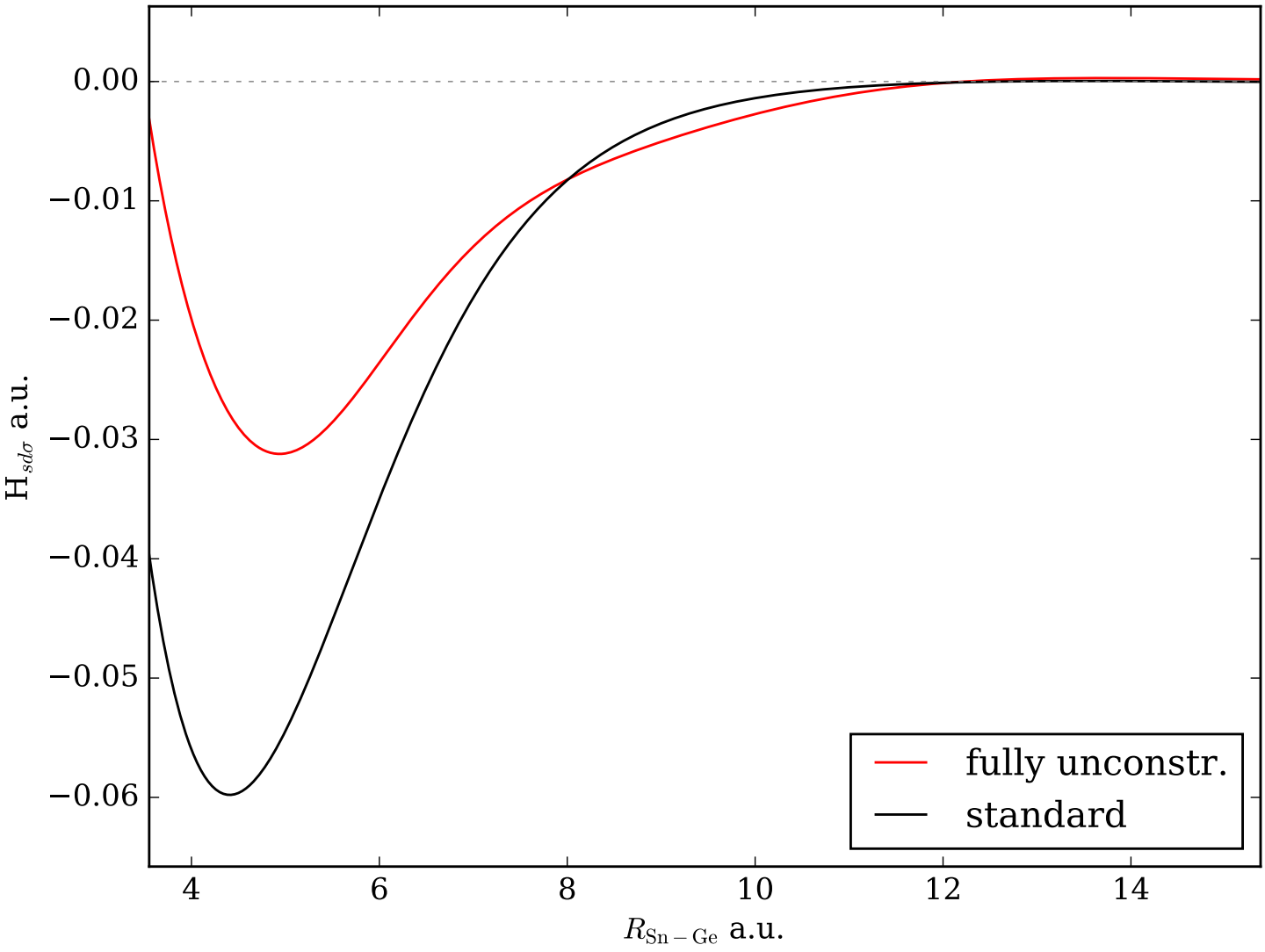

0.000
−0.005
−0.010
−0.015
−0.020
−0.025
−0.030
$H_{dd\delta}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Ge}}$ a.u.
fully unconstr.
standard

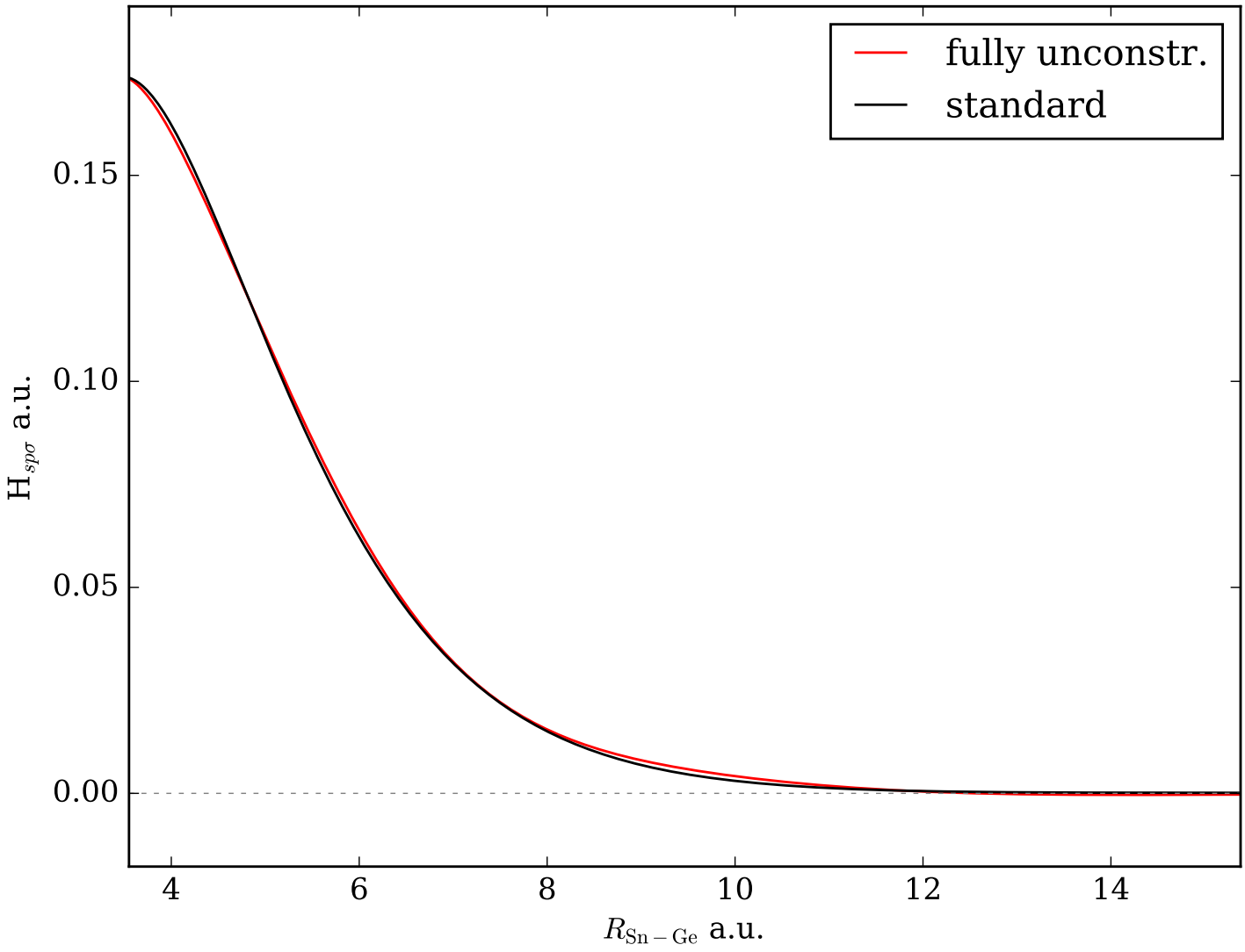

fully unconstr.
standard
0.02
0.01
0.00
−0.01
−0.02
−0.03
−0.04
−0.05
$H_{pd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Ge}}$ a.u.

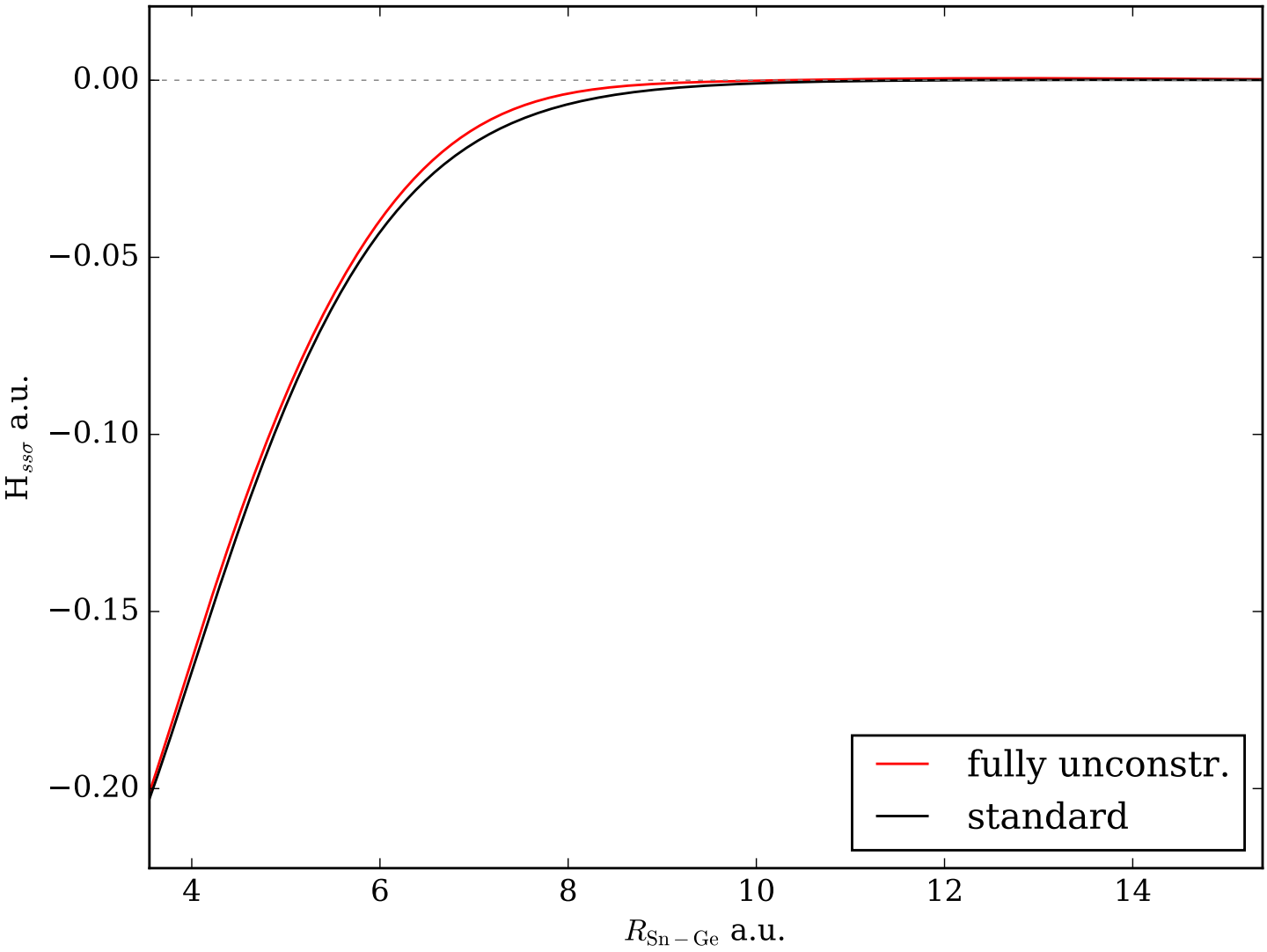

fully unconstr.
standard
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
$H_{pd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Ge}}$ a.u.

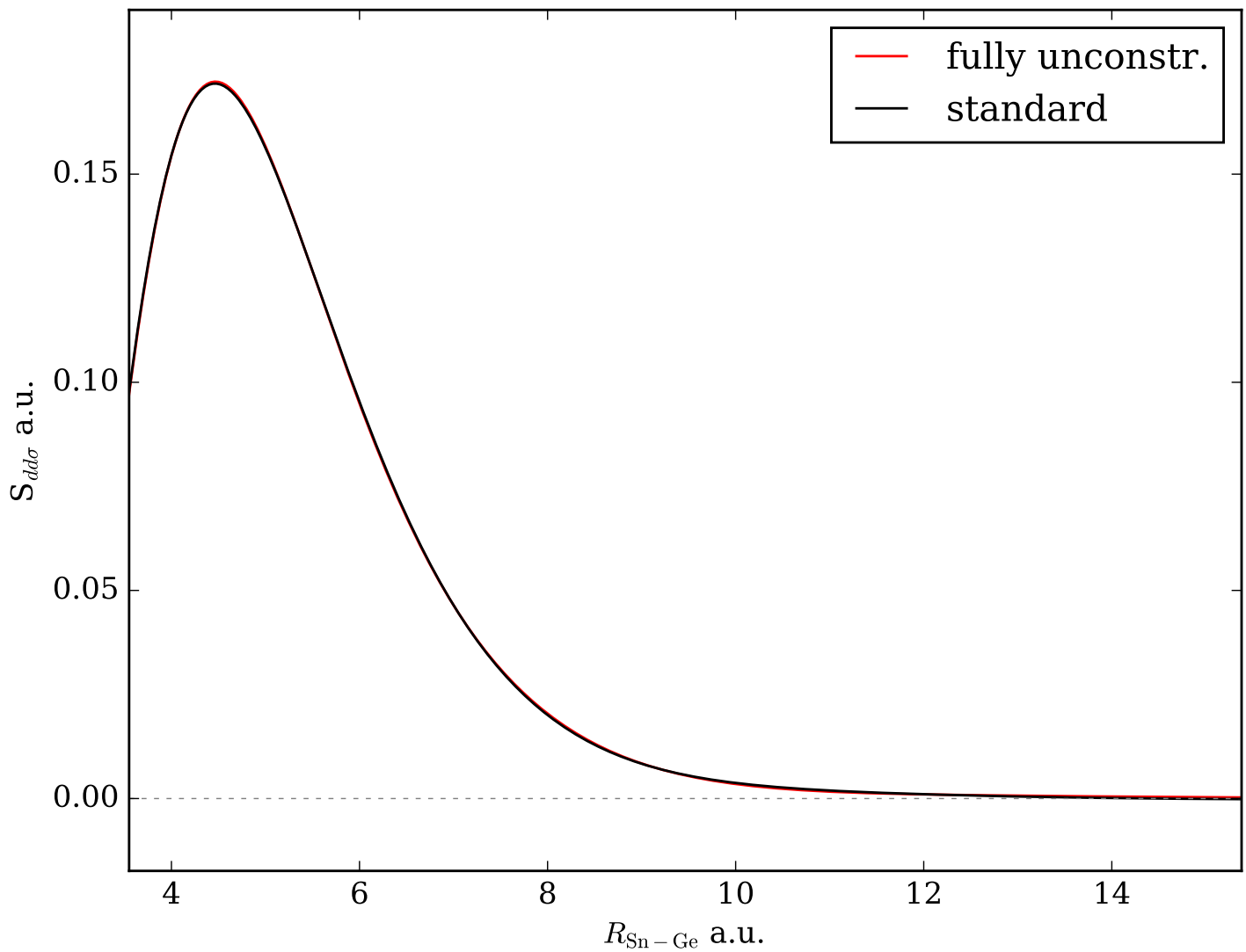

fully unconstr.
standard
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
$H_{pp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Ge}}$ a.u.

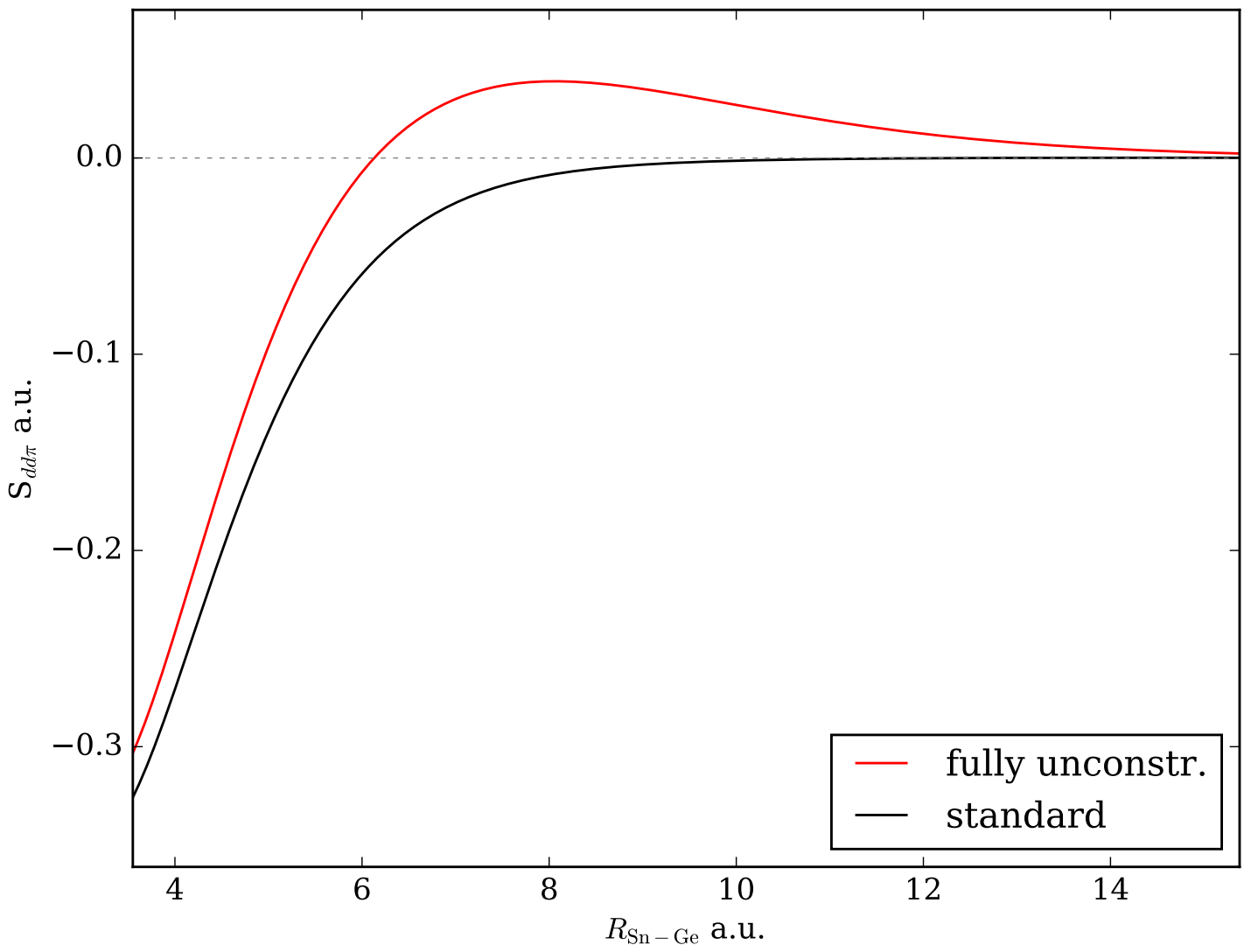

0.00
−0.02
−0.04
−0.06
−0.08
−0.10
−0.12
$H_{pp\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Ge}}$ a.u.
fully unconstr.
standard

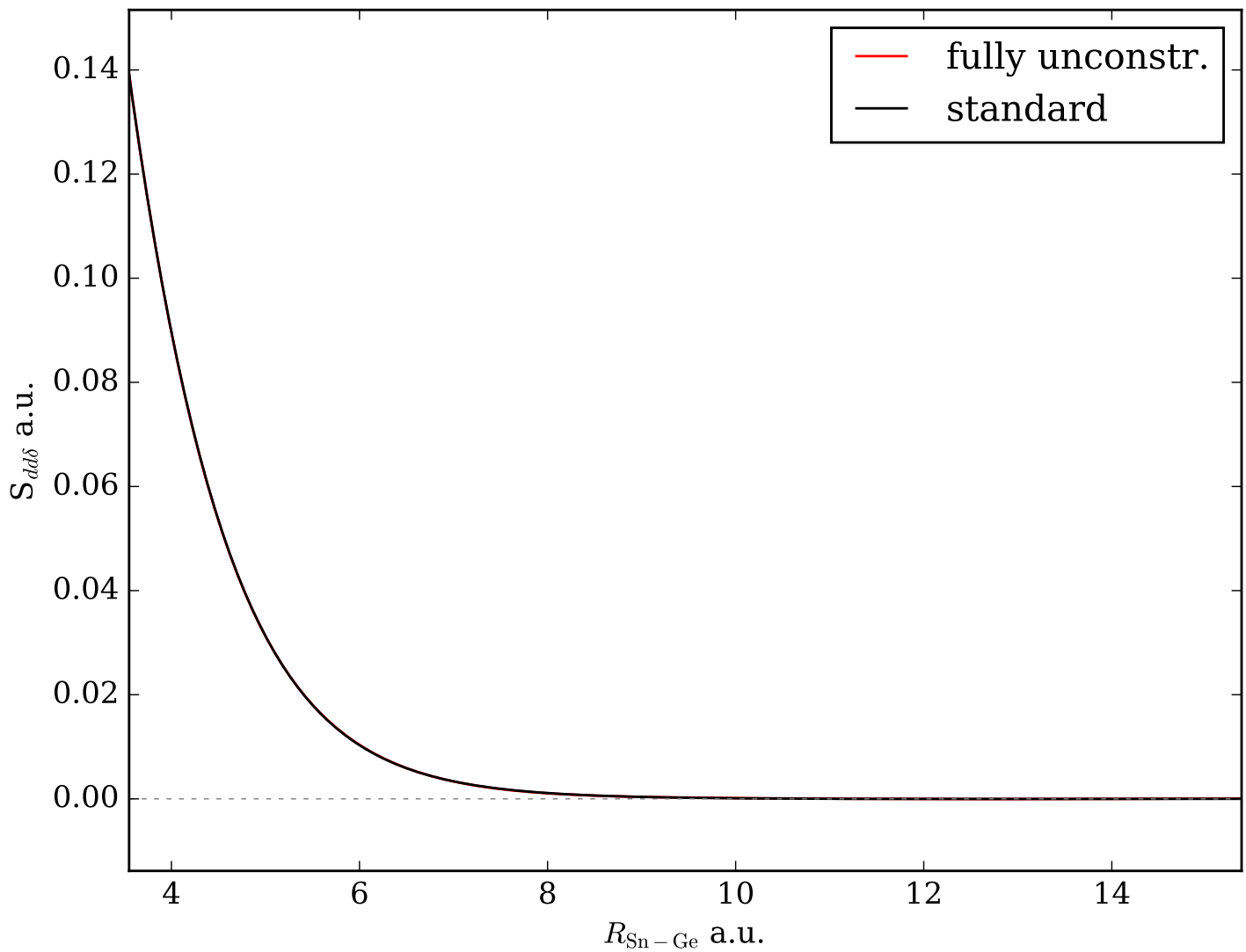

0.00
−0.01
−0.02
−0.03
−0.04
−0.05
−0.06
$H_{sd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Ge}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.15
0.10
0.05
0.00
$H_{sp\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Ge}}$ a.u.


0.00
−0.05
−0.10
−0.15
−0.20
$H_{ss\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Ge}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
0.15
0.10
0.05
0.00
$S_{dd\sigma}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Ge}}$ a.u.


0.0
−0.1
−0.2
−0.3
$S_{dd\pi}$ a.u.
4
6
8
10
12
14
$R_{\mathrm{Sn-Ge}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
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0.08
0.06
0.04
0.02
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4
6
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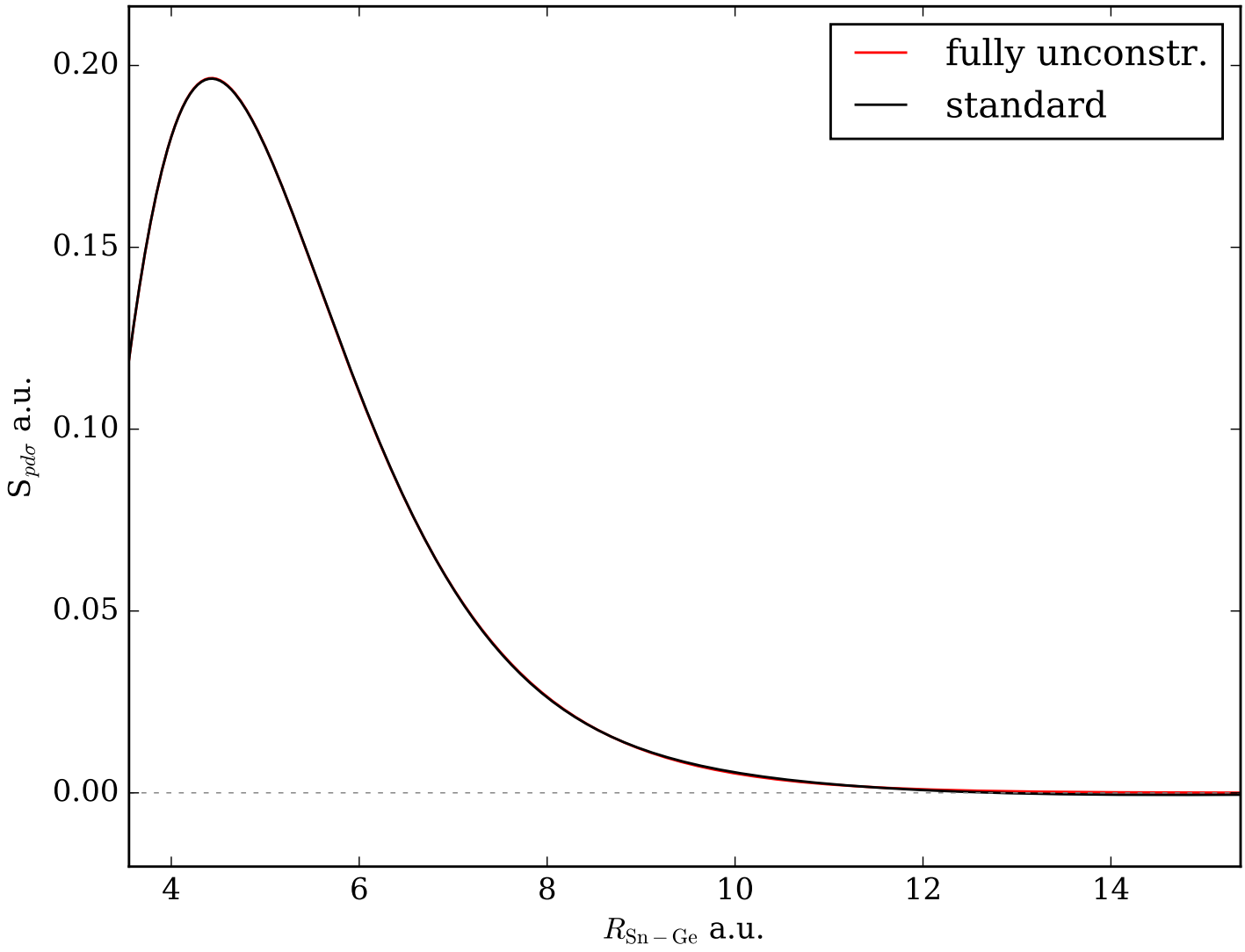
10
12
14
$R_{\mathrm{Sn-Ge}}$ a.u.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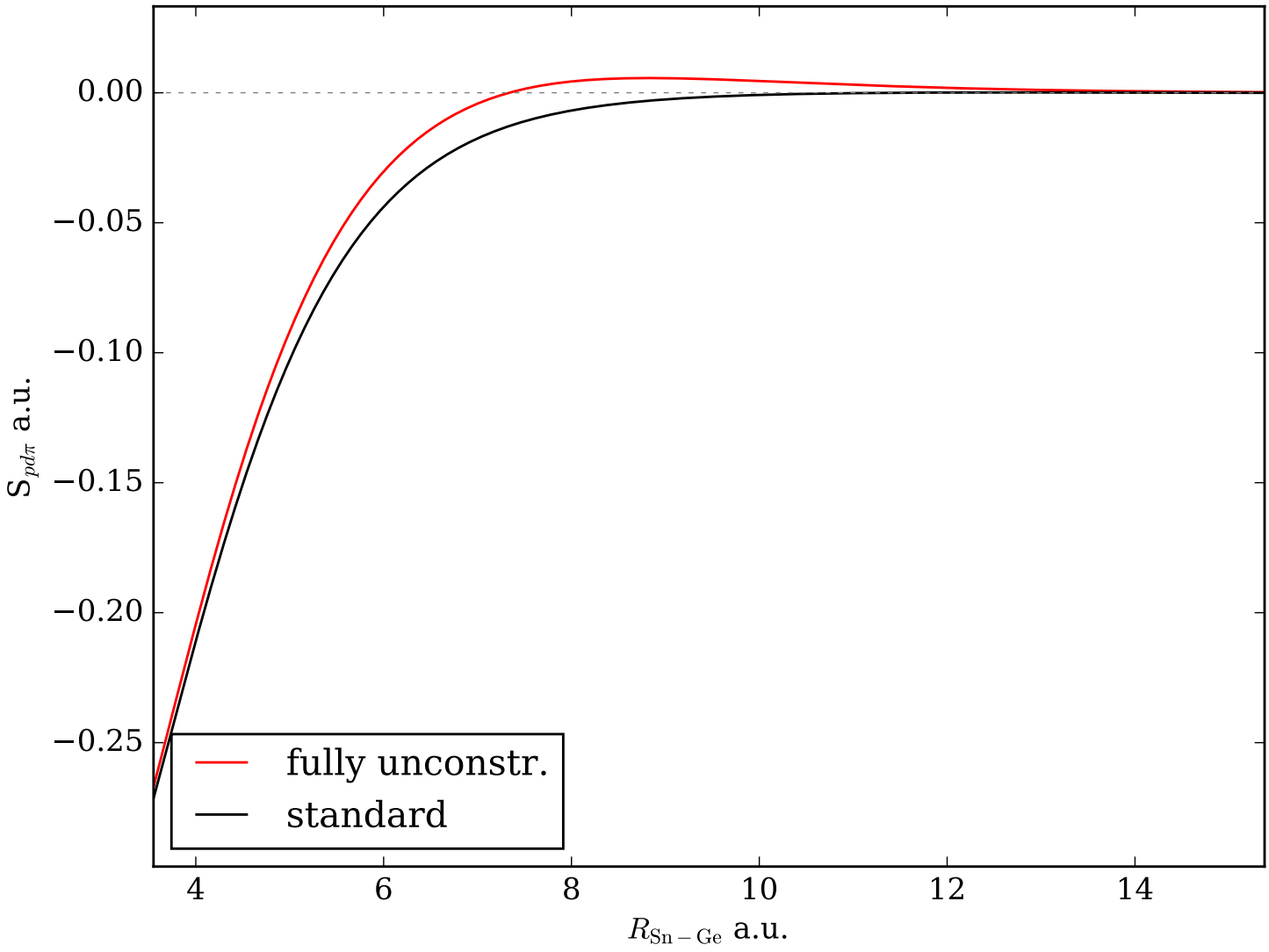
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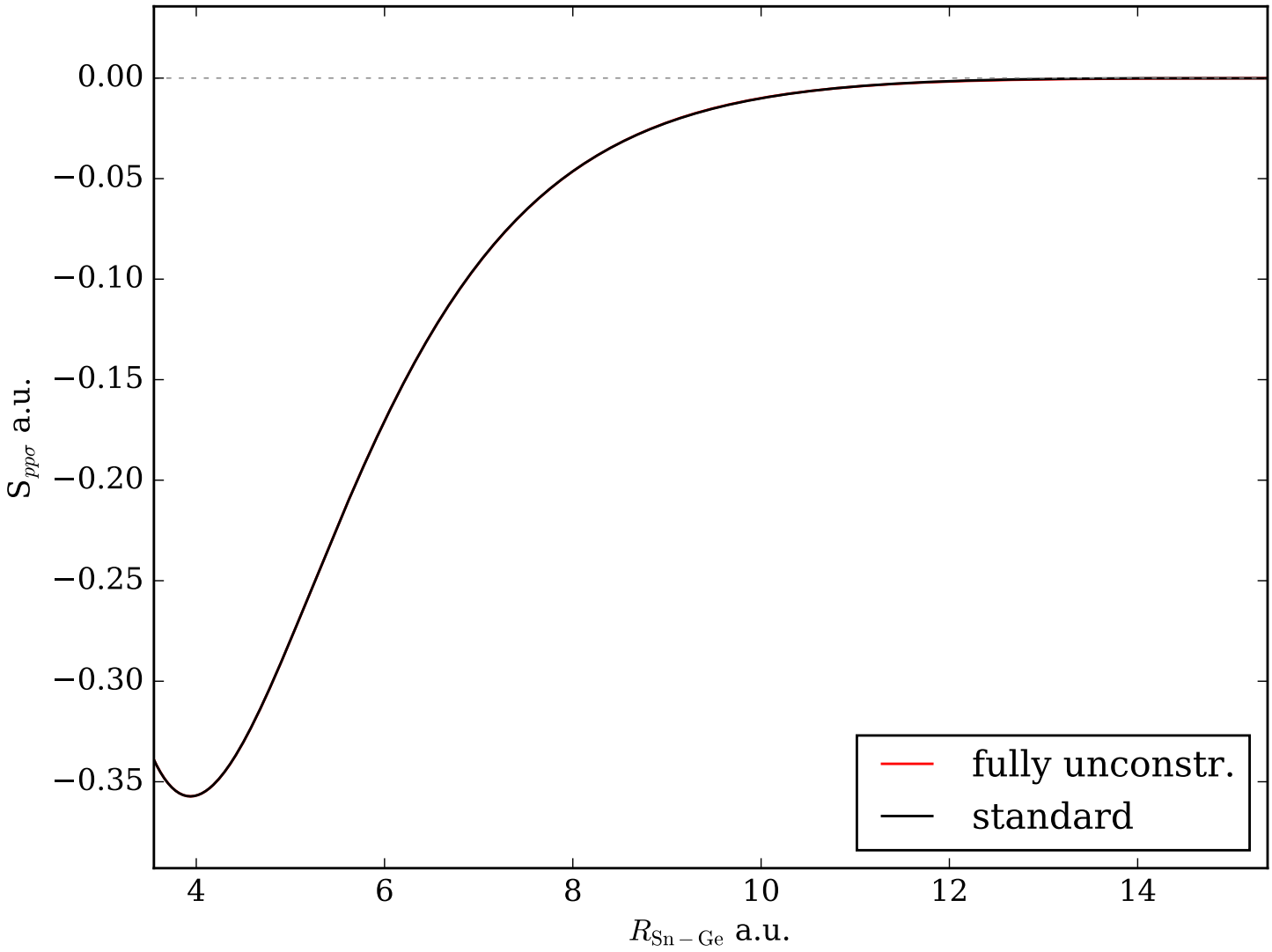
$R_{\mathrm{Sn-Ge}}$ a.u.
fully unconstr.
standard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$R_{\mathrm{Sn-Ge}}$ a.u.
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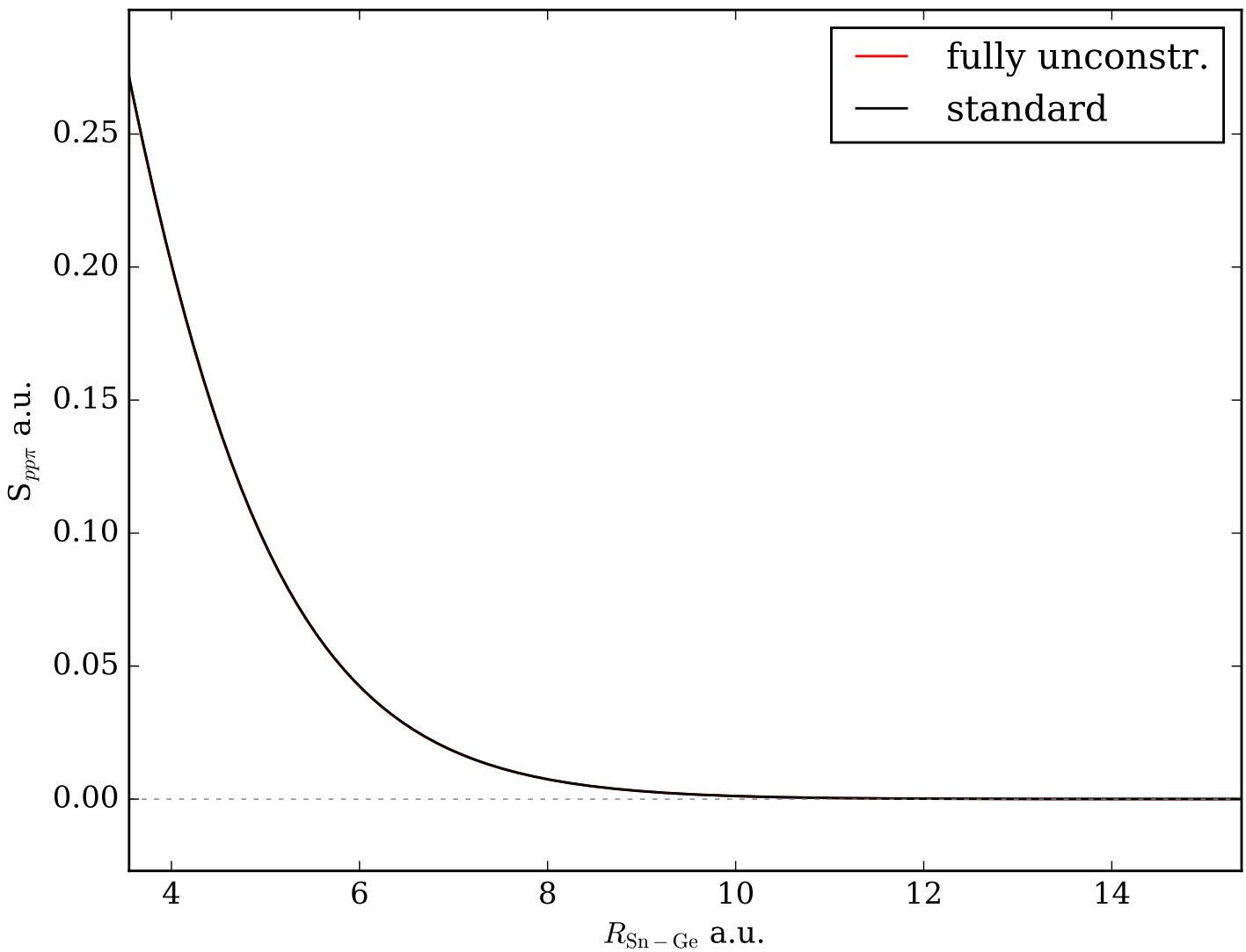
standard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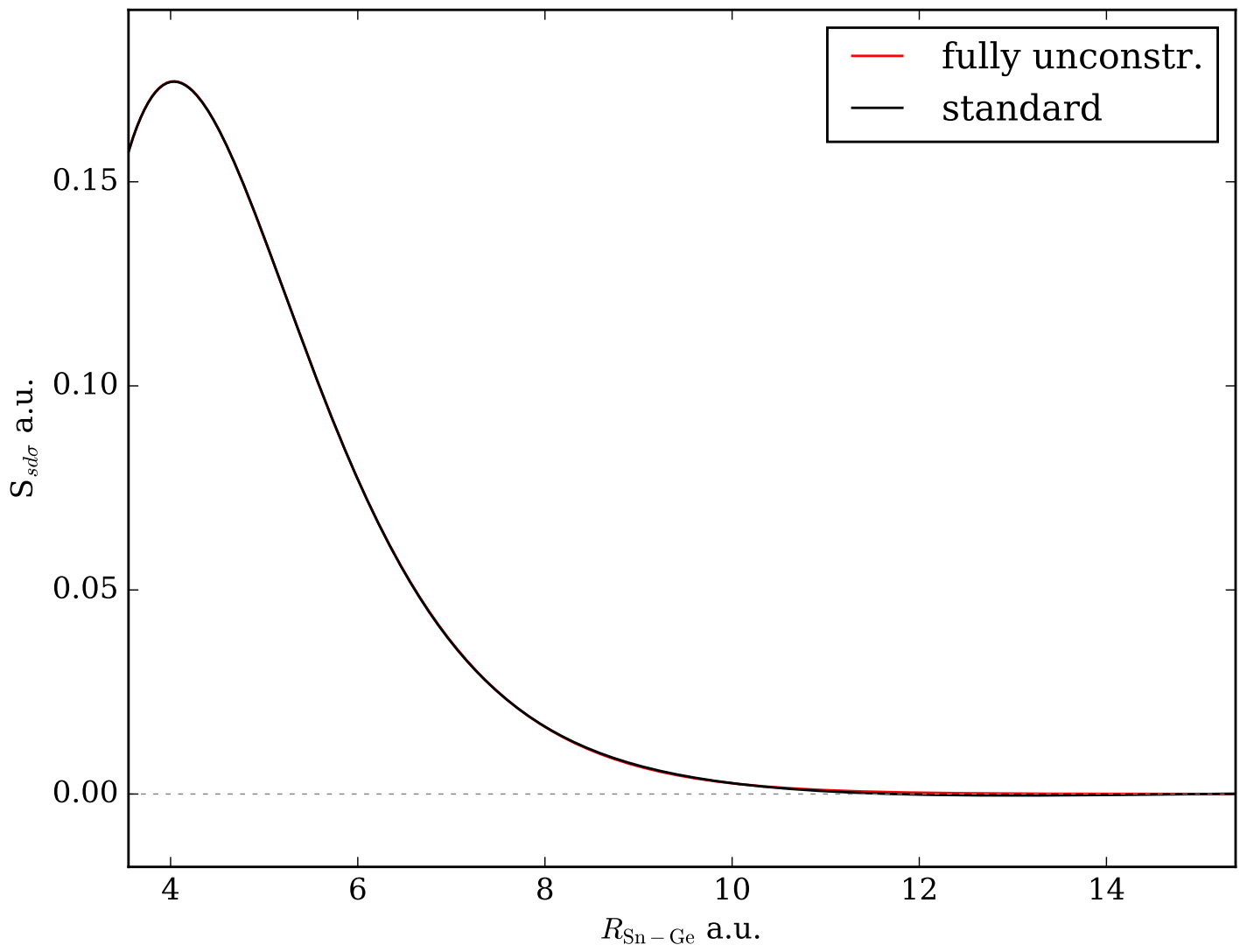
14
$R_{\mathrm{Sn-Ge}}$ a.u.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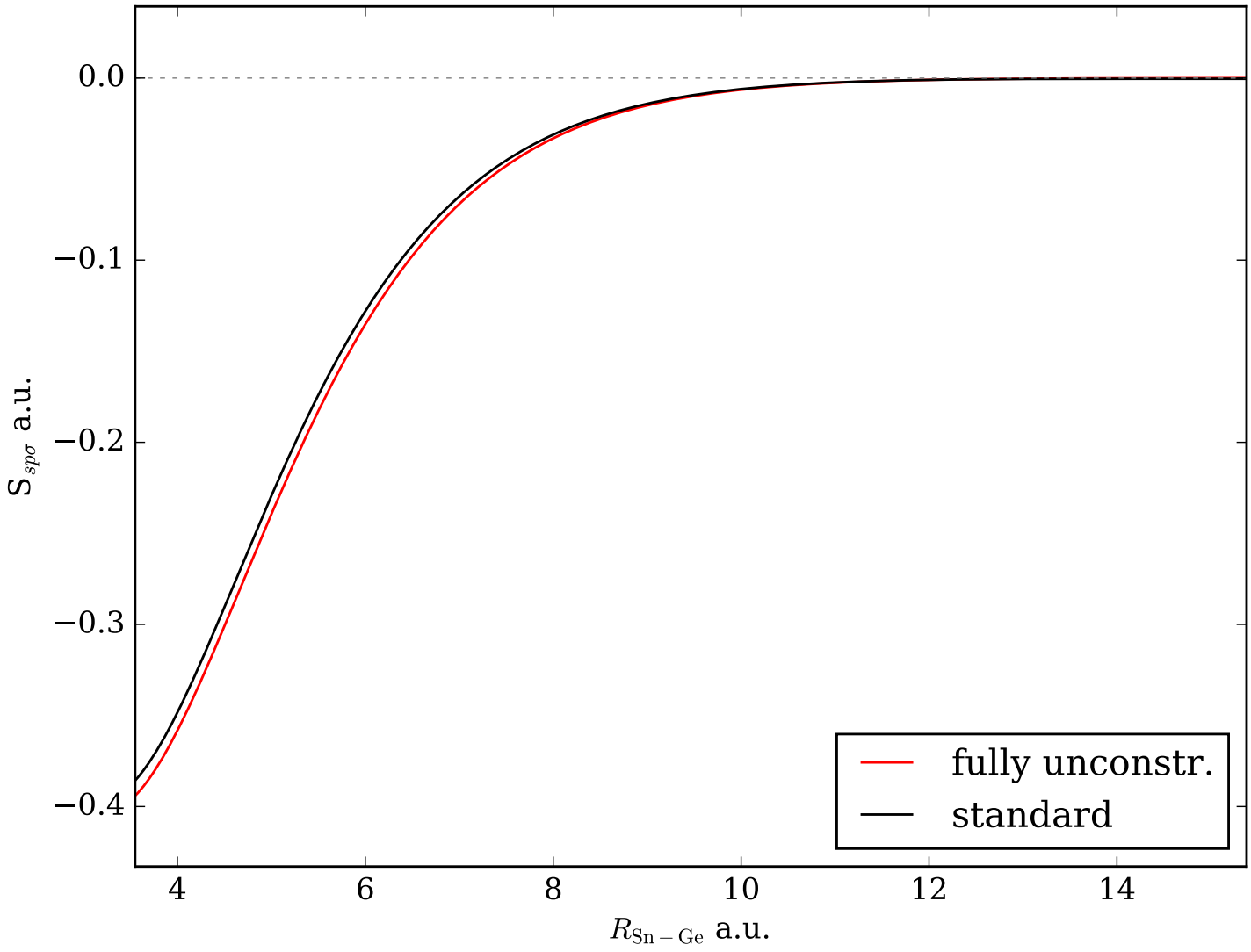
12
14
$R_{\mathrm{Sn-Ge}}$ a.u.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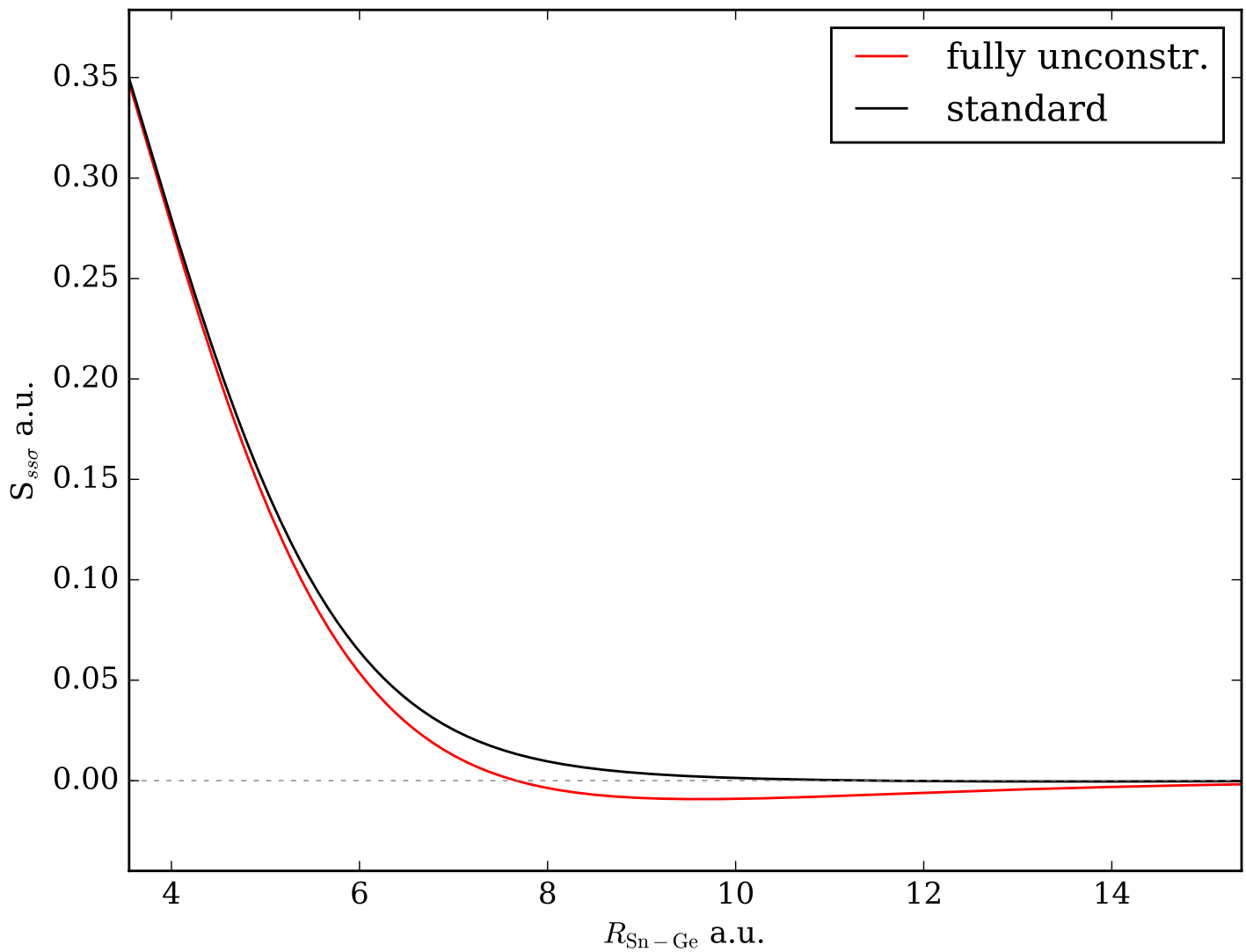
10
12
14
$R_{\mathrm{Sn-Ge}}$ a.u.
fully unconstr.
standard


fully unconstr.
standard
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0.10
0.05
0.00
$S_{ss\sigma}$ a.u.
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6
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10
12
14
$R_{\mathrm{Sn-Ge}}$ a.u.