

SUPPORTING INFORMATION

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Unmasking Static Correlation Error in Hybrid Kohn-Sham Density
Functional Theory

Dayou Zhang and Donald G. Truhlar

*Department of Chemistry, Chemical Theory Center, and Minnesota Supercomputing Institute,
University of Minnesota, Minneapolis, Minnesota 55455-0431, United States*

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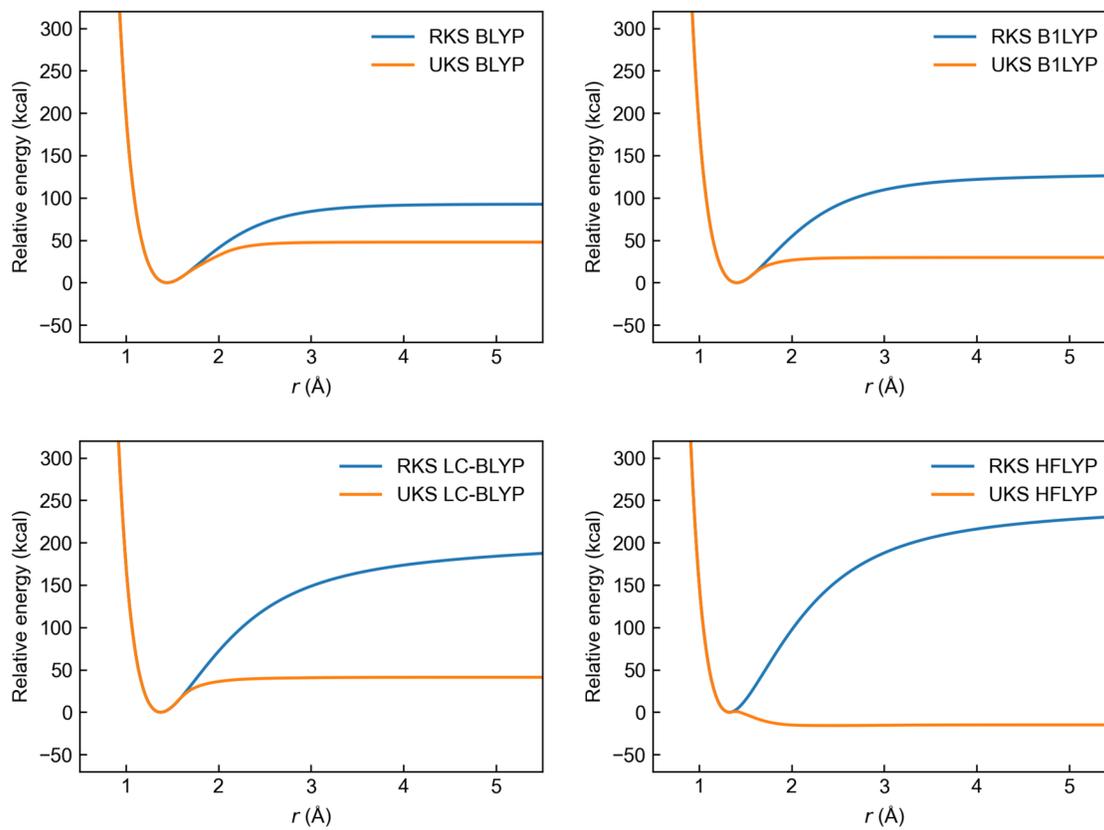


Figure S1 RKS and UKS potential energy curves for F_2 with BLYP, B1LYP, LC-BLYP, and HFLYP functionals

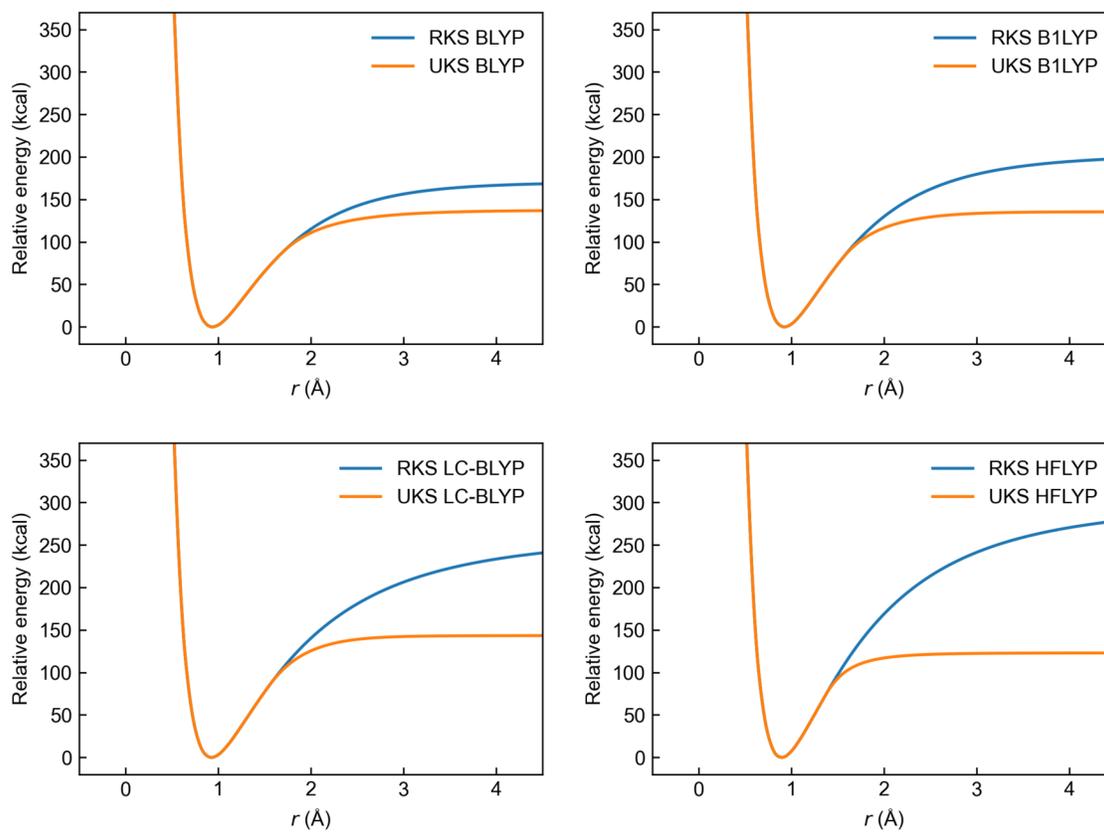


Figure S2 RKS and UKS potential energy curves for HF with BLYP, B1LYP, LC-BLYP, and HFLYP functionals

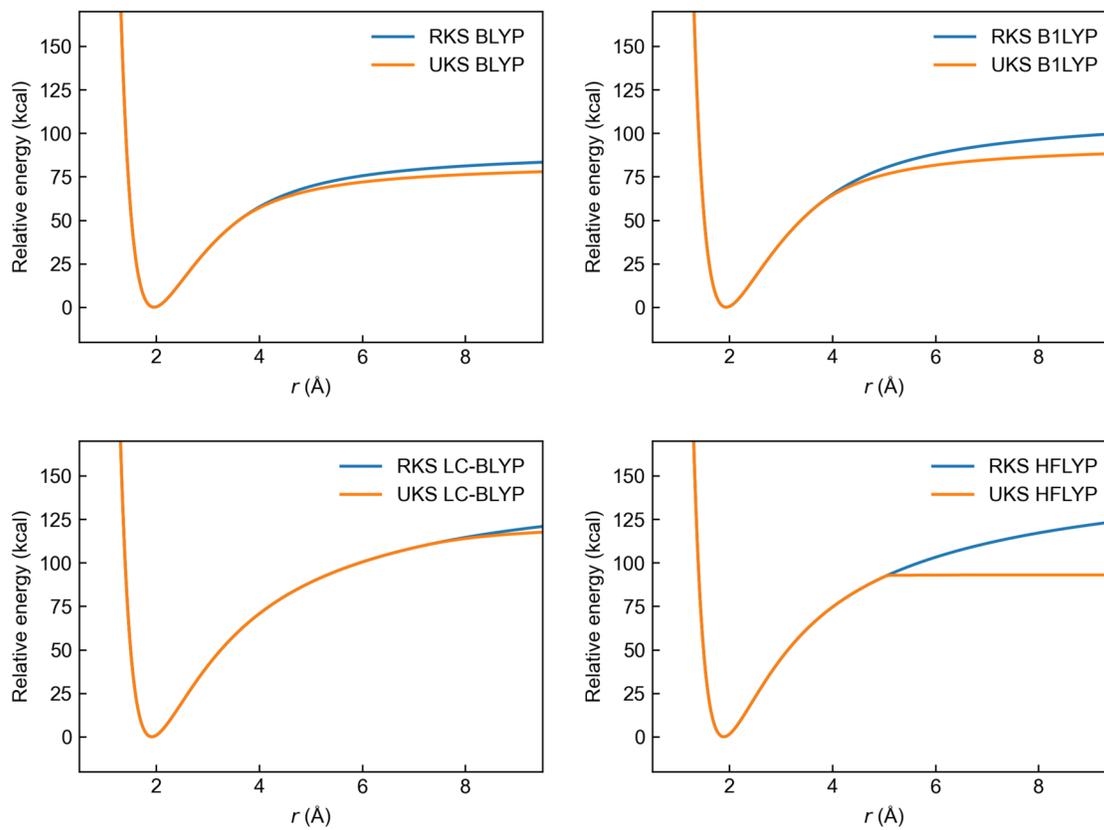


Figure S3 RKS and UKS potential energy curves for NaF with BLYP, B1LYP, LC-BLYP, and HFLYP functionals

Sample *Gaussian 16* input files

The following input file performs a single point calculation of H₂ using unrestricted HFLYP functional.

```
# stable(opt) UBLYP/6-31+g(d,p) int(grid=ultrafine,acc2e=12)
# IOp(3/76=0000010000) guess(read)
```

H2

0 1

H

H

1

B1

B1

0.7

The following input file performs a single point calculation of H₂ using unrestricted HLE16 functional.

```
# stable(opt) UHCTH407/6-31+g(d,p) int(grid=ultrafine,acc2e=12)
# IOp(3/76=1250000000) IOp(3/77=1000010000) IOp(3/78=0500005000)
# guess(read)
```

H2

0 1

H

H

1

B1

B1

0.7