

Supporting Information for: X-Ray Absorption in Insulators with Non-Hermitian Real-Time Time-Dependent Density Functional Theory

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Si₅O₁₆H₁₂ cluster geometry in Å

Si	0.39221095	-0.03543176	0.05250489
O	1.80641918	-0.77521497	0.03083506
O	0.11442704	0.58372974	-1.40835065
O	0.43329849	1.14856662	1.13436654
O	-0.78612236	-1.05242084	0.46010557
Si	2.29588684	-2.33661876	0.24409997
Si	-0.59982064	1.80266507	-2.23308277
Si	0.34312850	2.42943860	2.11196954
Si	-2.04085654	-1.87020620	-0.21097811
O	2.30009761	-2.51114198	1.92497222
O	1.33366440	-3.40293144	-0.59881184
O	3.87900065	-2.53963593	-0.30965559
H	2.70404213	-3.28465360	2.41334564
H	0.34094817	-3.40039204	-0.71926113
H	4.07567371	-2.94004598	-1.20463687
O	-0.55735642	3.24403271	-1.41826939
O	-2.17076839	1.17392378	-2.51521853
O	0.03259483	2.03256523	-3.77389560
H	-0.51732211	3.44341018	-0.43916476
H	-2.76974293	1.54390341	-3.22539074
H	0.69984036	2.74264443	-3.99877542
O	-0.68717913	2.28778142	3.42334432
O	1.85026020	2.85468925	2.71719749
O	-0.36249213	3.63603523	1.12801832
H	-0.42455275	1.95121633	4.32764036
H	2.73086988	2.75778665	2.25336941
H	-0.78386532	4.45758924	1.51206733
O	-3.08779838	-2.51061246	0.94111731
O	-2.91670902	-0.95523054	-1.27656949
O	-1.24797830	-3.22733021	-0.89119877
H	-3.95258790	-2.07564465	1.19199993
H	-2.66075458	-0.14754288	-1.80772669
H	-1.74183970	-4.01726835	-1.25465253