Supporting Information

First Hybrid Embedding Scheme for Polar Covalent Materials Using an Extended Border Region to Minimize Boundary Effects on the Quantum Region

Alexei M. Shor, Elena A. Ivanova Shor, Vladimir A. Nasluzov,
Georgi N. Vayssilov, Notker Rösch

Table S1. Optimized Gaussian-type orbital exponents (au) the of border centers O*.

s	P	d
42.9945813397	44.1800166163	1.5876992947
15.4994950057	10.0730313065	
6.2258536472	2.65650061594	
1.0239161449	0.73353152694	
0.3209359861	0.17372185997	

Table S2. Optimized pseudopotential parameters[a] (au) of the border centers O* and Si^{PP}*.

	l	k	α_{kl}	A_{kl}
O*	0	1	26.023166	78.753643
	0	2	14.897082	15.444531
	1	1	23.555342	-15.348110
	1	2	13.256028	3.112648
	2	1	0.027616	-0.001791
Si^{PP}*	0	1	1.756846	6.581120
	1	1	0.882640	2.048685
	2	1	0.943234	-2.036544

[a] For the analytical form of the pseudopotential, see Eq. (1).

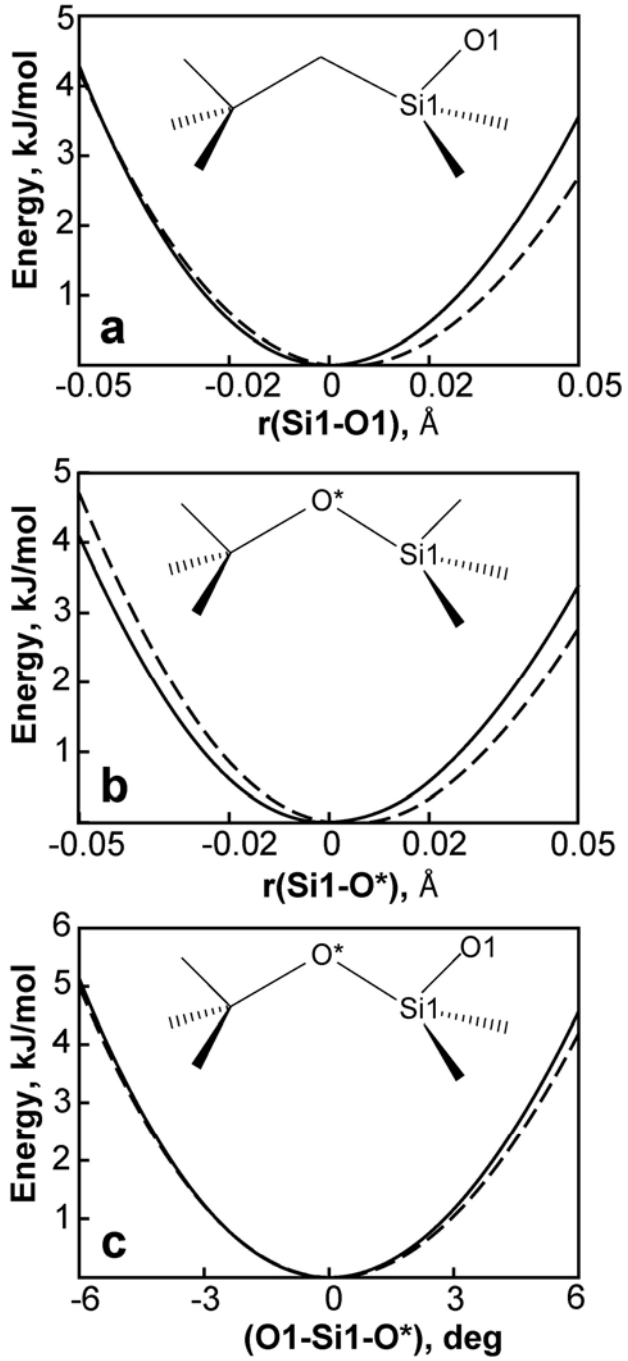

Figure S1. Comparison of various potential energy curves: (a) Si1-O1 bond, (b) Si1-O* bond, and (c) O1-Si1-O* angle in the systems shown in Fig. 2: reference (QM; dashed line) and target (QM/MM; solid line). The curves were obtained by varying (a) the bond lengths Si1-O1, (b) Si1-O* and (c) the bond angle O1-Si1-O*, keeping all other internal coordinates fixed at their values as optimized for the reference system.