Novel high- κ dielectrics for next-generation electronic devices screened by automated *ab initio* calculations

Kanghoon Yim^{1,2}, Youn Yong^{1,2}, Joohee Lee^{1,2}, Kyuhyun Lee^{1,2}, Ho-Hyun Nahm^{3,4}, Jiho Yoo⁵, Chanhee Lee⁵, Cheol Seong Hwang^{1,2} & Seungwu Han^{1,2,*}

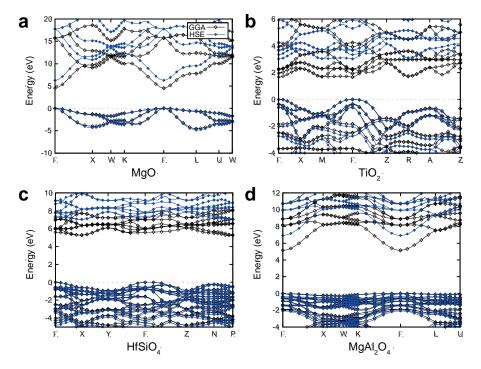


Figure S1. Comparison of GGA and HSE06 band structures for some oxides. The rigid shift between the bands are noticeable.

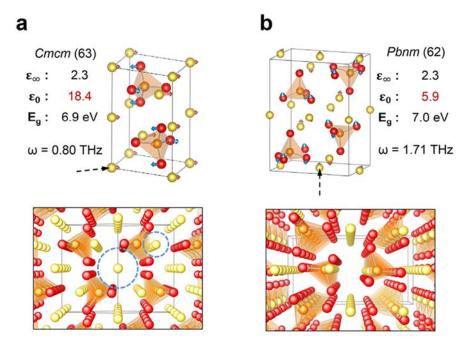


Figure S2. a) *Cmcm* and b) *Pbnm* phases of Na₂SO₄. The atomic arrangements viewed along the dashed arrows are shown at the bottom. The dashed circles in a) show the unblocked channel along which Na atoms can oscillate in large amplitudes.