Computational Screening for Sustainable Two-dimensional Ultra-wide Bandgap Materials

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Abstract

Presently used ultra-wide bandgap semiconductors comprise predominantly bulk materials, but their large size, high power and high cost is an obstacle to meeting the future requirements of high-performance (opto)electronic devices [1]. Ultra-wide bandgap two-dimensional materials serve as a promising solution to meet these needs. While the rise of materials databases specific to two-dimensional materials provides us with many options to choose from, various considerations, such as the difficulty of synthesizing these materials and the fact that certain elements are under serious supply threat in the near future while some others are environmentally harmful [2, 3], complicate how we choose new candidate materials for such applications. We devised a strategy to screen for sustainable, easily exfoliable and stable candidate two-dimensional materials from the 2DMatPedia database [4] for various (opto)electronic applications. We assessed the screened candidate materials for their performance in specific (opto)electronic device applications using density functional theory (DFT) and related first-principles methods. The properties computed include the HSE06 band alignments, optB88 static dielectric constants and GW-BSE optical spectra, besides some properties from transport simulations. These calculations inform us of the potential for these candidate materials to be used as transistor materials, specifically gate dielectrics and channel materials, as well as for (polarization-sensitive) ultraviolet photodetection.

References

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