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Ab initio calculation of natural band offsets of all group IV, II-VI and III-V semiconductors SU-HUAI WEI, ARON WALSH, National Renewable Energy Laboratory, YONG-HUA LI, XINGAO GONG, Fudan University — The natural band offset between semiconductors is one of the most fundamental properties in materials physics. It is a necessary quantity to assess charge transport and quantum confinement, and is of particular relevance to the design of optoelectronic devices which feature an interface between two or more materials. However, in the past, the natural band offset calculations were based on the assumption that certain reference levels (core levels, average Coulomb potentials, etc.) have zero absolute deformation potential, and thus align between the bulk and heterostructures. In this study [1], using an all-electron band structure approach, we have systematically calculated the natural band offsets between all group IV, III-V and II-VI semiconductor compounds, taking into account the deformation potential of the core states. This revised approach removes assumptions regarding the deformation potential of the reference levels, and offers a more reliable prediction of the 'natural' unstrained offsets. Comparison is made to experimental work, where a noticeable improvement is found compared to previous methodologies. [1] Y.-H. Li et al., Appl. Phys. Lett. **94**, 212109 (2009).

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