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Absolute surface energy calculations of Wurtzite (0001)/(000-1): a study of ZnO and GaN[1] JINGZHAO ZHANG, YIOU ZHANG, KINFAI TSE, BEI DENG, Chinese Univ of Hong Kong, HU XU, South University of Science and Technology of China, JUNYI ZHU, Chinese Univ of Hong Kong — The accurate absolute surface energies of (0001)/(000-1) surfaces of wurtzite structures are crucial in determining the thin film growth mode of important energy materials. However, the surface energies still remain to be solved due to the intrinsic difficulty of calculating dangling bond energy of asymmetrically bonded surface atoms. We used a pseudo-hydrogen passivation method to estimate the dangling bond energy and calculate the polar surfaces of ZnO and GaN. The calculations were based on the pseudo chemical potentials obtained from a set of tetrahedral clusters or simple pseudo-molecules, using density functional theory approaches, for both GGA and HSE. And the surface energies of (0001)/(000-1) surfaces of wurtzite ZnO and GaN we obtained showed relatively high self-consistencies. A wedge structure calculation with a new bottom surface passivation scheme of group I and group VII elements was also proposed and performed to show converged absolute surface energy of wurtzite ZnO polar surfaces.

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Jingzhao Zhang
Chinese Univ of Hong Kong

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