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Tetrahedral cluster and pseudo molecule: New approaches to Calculate Absolute Surface Energy of Zinc Blende (111)/(-1-1-1) Surface[1]
YIOU ZHANG, JINGZHAO ZHANG, KINFAI TSE, LUN WONG, CHUNKAI CHAN, BEI DENG, JUNYI ZHU, Chinese Univ of Hong Kong — Determining accurate absolute surface energies for polar surfaces of semiconductors has been a great challenge in decades. Here, we propose pseudo-hydrogen passivation to calculate them, using density functional theory approaches. By calculating the energy contribution from pseudo-hydrogen using either a pseudo molecule method or a tetrahedral cluster method, we obtained (111)/(-1-1-1) surfaces energies of Si, GaP, GaAs, and ZnS with high self-consistency. Our findings may greatly enhance the basic understandings of different surfaces and lead to novel strategies in the crystal growth.

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Yiou ZHANG
Chinese Univ of Hong Kong

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