

Supplementary Material

First principles study of the photoelectric properties of alkaline earth metal (Be/Mg/Ca/Sr/Ba)-doped monolayers of MoS₂

Li-Zhi Liu, Xian-Sheng Yu, Shao-Xia Wang, Li-Li Zhang, Xu-Cai Zhao, Bo-Cheng Lei and Hong-Mei Yin, Yi-Neng Huang

1. Convergence test

In order to greatly reduce the calculation time on the basis of accurate calculation, convergence tests were carried out on the supercell size of MoS₂, cutoff energy of geometric optimization calculation and K-lattice points, as shown in Figure 1 (a), (b) and (c) respectively. As can be seen from Figure 1 (a), the supercell starts from 2×2×1, the energy of the system decreases somewhat and tends to be gentle. However, considering the large supercell energy is closer to the properties of the materials under study, 4×4×1 MoS₂ was selected as the research object on the basis of stable energy and sufficient computing resources. As can be seen from Figure 1 (b) and (c), when the truncation energy and K grid points were 450 eV and 5×5×1, the system energy decreases somewhat and tends to be flat. Therefore, we have used a cutoff energy of 450 eV and 5×5×1 K-points grid for all the calculations.

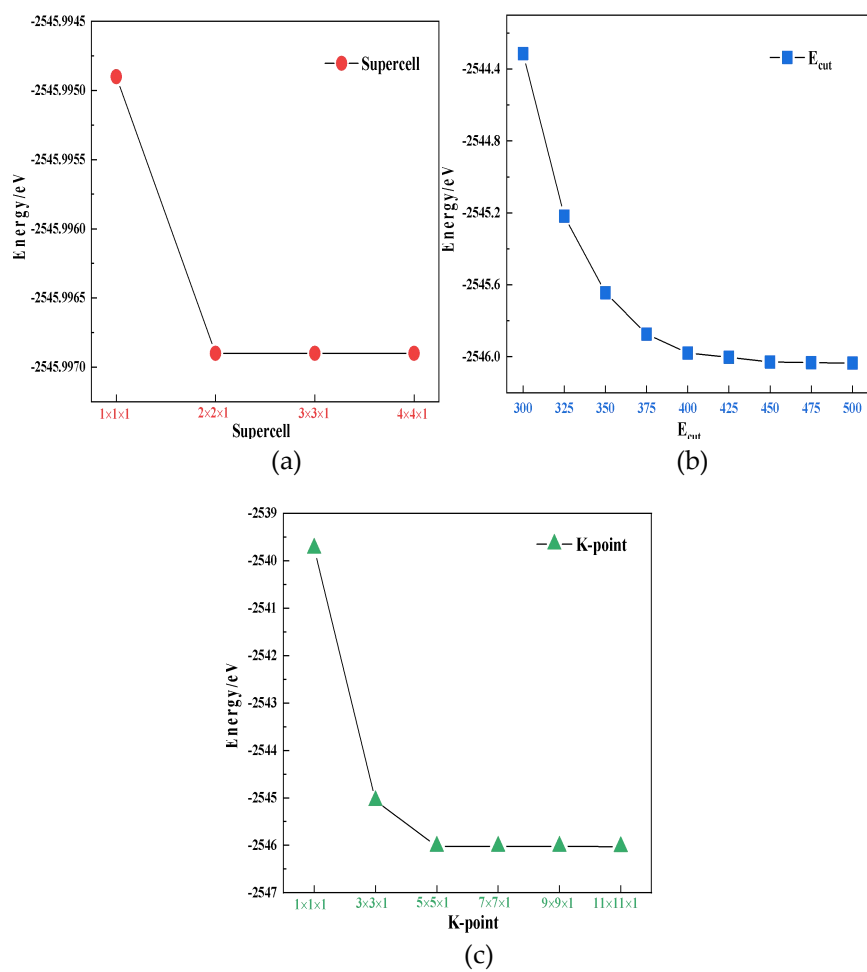


Figure S1 Convergence tests of MoS₂

(a) Convergence test of supercell; (b) Convergence test of cutoff energy; (c) Convergence test of K-point;