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First-principles electronic structure of β-$FeSi_2$ and FeS_2 surfaces[1]
PENGXIANG XU, TIMO SCHENA, STEFAN BLÜGEL, GUSTAV BIHLMAYER, Peter Gruenberg Institut & Institute for Advanced Simulation, Forschungszentrum Juelich and JARA, 52425 Juelich, Germany — Applying density functional theory in the framework of the full-potential linearized augmented plane-wave (FLAPW) method [1], we investigated electronic structure of potential future photovoltaic materials, β-$FeSi_2$ and FeS_2, for selected surface orientations and terminations. The most stable orientations are determined by comparing their surface energy. Detailed electronic structure calculations show that surface states originating from Fe play an important role and might determine photovoltaic properties. Our results show that anti-ferrimagnetic ordering exists for Fe-terminated surface. Furthermore, we also studied how electronic structure and photovoltaic efficiency are affected by the recently observed structural defects such as stacking fault in β-$FeSi_2$.

[1] www.flapw.de

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