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First-principles electronic structure of β-$FeSi_2$ and FeS_2 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 in their bulk phases and for selected surface orientations and terminations. Their band gaps are examined using hybrid functionals as well as many-body perturbation theory in the GW-approximation to get insight of their photovoltaic performance. The gap nature in β-$FeSi_2$ changes from direct to indirect as suitable stain field is induced in the structure by epitaxially matching with Si substrate. Furthermore, we also studied the atomic and electronic structure of β-$FeSi_2$ and FeS_2 thin films for different orientations with different terminations. The most stable orientations are determined by comparing their cohesive energy. Detailed electronic structure calculations show that surface states originating from Fe play an important role and might determine their photovoltaic properties.

[1] www.flapw.de

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