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Theoretical study on the possibility of S doping in anatase TiO_2[1]
YUTING PENG, JIAO AN, QIMING ZHANG, Univ of Texas, Arlington — Titanium dioxide (TiO_2) is well known for its numerous and diverse applications. Usually doping is often used to tune the properties of materials. In this work, isovalent Sulfur (S) doping in anatase TiO_2 ($TiO_{2-x}S_x$) was studied using the first principles method. The total energy calculations were used to determine the defect formation energies and the chemical potential landscape with different S doping concentrations. The results showed that anatase $TiO_{2-x}S_x$ with concentrations x=0.0278 and 0.0625 cannot exist without the co-existence of other Ti binary compounds, such as TiO_2, Ti_2O_3, TiS, TiS_2, and TiS_3. Moreover, other elements doped with S together to stabilize the compounds were also investigated.

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