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Theoretical prediction of stable tin oxides: stoichiometry, electronic structure and possible applications JUNJIE WANG, NAOTO UMEZAWA, National Institute for Materials Science, THEORETICAL DESIGN OF ENVIRONMENTAL REMEDIATION MATERIALS TEAM — We have carried out a computational materials search for stable crystal phases of tin oxides in different composition ratios under ambient pressure condition. By employing density-functional theory calculations combined with evolutionary algorithm, we have identified several thermodynamically stable phases of tin oxides and investigated their dynamical stabilities by computing phonon vibration frequencies. We revealed the mechanism of determining the electronic structures of tin oxide crystals/van der Waals heterostructures through a systematic computational study of chemical bonding, band structure and Bader charges. Based on our theoretical analysis, we demonstrated that the predicted structures can lead to a desirable band structure for photocatalytic hydrogen evolution from water solution. Therefore, the tin oxides proposed in the present work have great potential as an abundant, cheap and environmentally-benign solar-energy conversion catalyst.

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