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Identifying the intermediate phase of tin oxides as Sn_3O_4 through Raman spectroscopy from theory and experiment MARCEL GIAR, BIANCA EIFERT, Institute of Theoretical Physics, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen, Germany, MARTIN BECKER, CHRISTIAN T. REINDL, I. Institute of Physics, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen, Germany, LILAN ZHENG, Faculty of Materials Science and Engineering, Hubei University, Wuhan 430062, China, ANGELIKA POLITY, I. Institute of Physics, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen, Germany, YUNBIN HE, Faculty of Materials Science and Engineering, Hubei University, Wuhan 430062, China, CHRISTIAN HEILIGER, Institute of Theoretical Physics, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen, Germany, PETER J. KLAR, I. Institute of Physics, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — The existence of an intermediate phase within the tin oxide system was first reported in 1882. However, its stoichiometry and its crystal structure have been dubious and heavily debated ever since, despite a multitude of structural investigations. Here we show that a combined Raman spectroscopic investigation based on *ab initio* methods and experiments offers an alternative to diffraction studies, which are not conclusive for this material system. It allows us to unambigiuously identify the intermediate phase as Sn_3O_4 and to rule out the other likely candidate, Sn_2O_3. We assign the one-phonon Raman signals of Sn_3O_4 to the mode symmetries of the corresponding point group C_{2h} and confirm the space group as $P2_1/c$ with 14 atoms per unit cell.

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