Optical properties of amorphous Zn-Sn-Ti oxides: A combined molecular dynamics and density functional theory study

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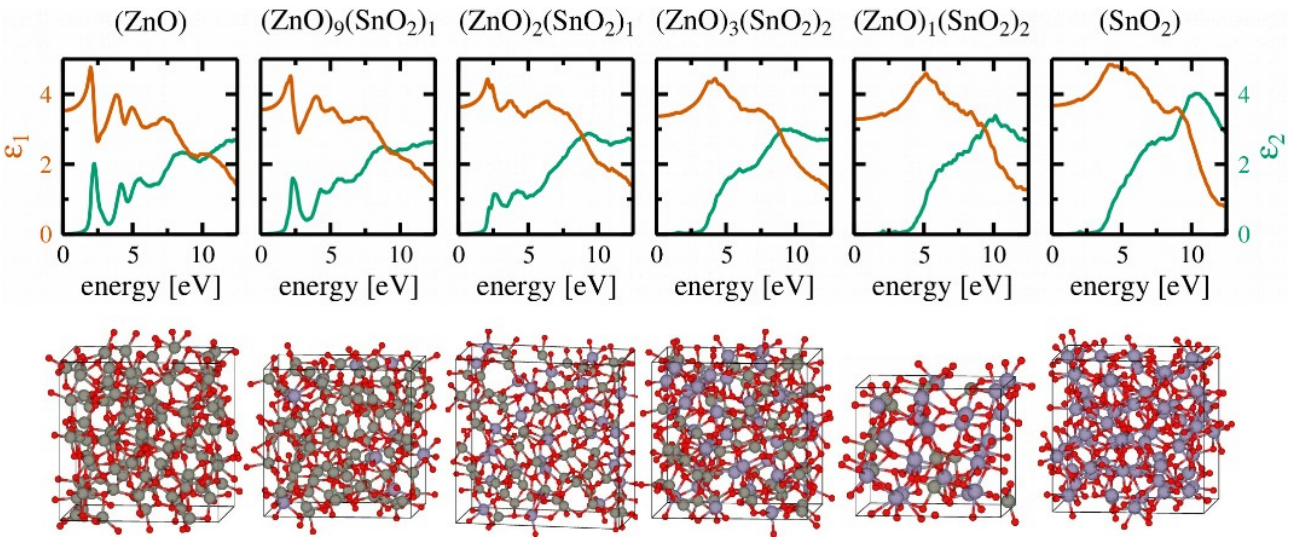
Amorphous transparent conducting oxides (TCOs) are widely used in technological applications due to their high transparancies, charge carrier mobilities, and flexibility. However, the up-to-now industry standard, amorphous In-Ga-Zn-O (a-IGZO), incorporates the rare and expensive indium, and active research is under way to find materials and/or material combinations to replace a-IGZO. A promising material combination with similar properties as a-IGZO has been identified within the $(ZnO)_x(SnO_2)_y(TiO_2)_z$ solid-solution. The immense parameter space for fabrication of this system (x:y:z ratio) makes computational screening and insights highly desirable.

Here, we report on our combined ab initio molecular dynamics (MD) and density functional theory (DFT) study of amorphous $(ZnO)_x(SnO_2)_y(TiO_2)_z$ solid-solutions. Covering the whole parameter space (x:y:z ratio) we generated amorphous structures using a well-established melt and quench approach. Some of the structures generated for the ternary $(ZnO)_x(SnO_2)_y$ solid-solution are shown in the lower panels of the figure. Based on the resultant structures, structural, electronic, and optical properties are analysed and compared with available experimental and theoretical data. The electronic properties are calculated using the hybrid HSE06 [1] and a self-consistent hybrid functional method [2], which has been proven to yield improved results for bulk oxide semiconductors [3]. The obtained dielectric functions for the ternary $(ZnO)_x(SnO_2)_y$ solid-solution are shown in the upper panels of the figure.



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