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High-throughput Screening and Statistical Learning for the Design of Transparent Conducting Oxides CHRISTOPHER SUTTON, LUCA GHIRINGHELLI, MATTHIAS SCHEFFLER, Fritz Haber Institute of the Max Planck Society — Transparent conducting oxides (TCOs) represent a class of well-developed and commercialized wide-bandgap semiconductors that are crucial for many electronic devices. Al, Ga, and In-based sesquioxides are investigated as new TCOs motivated by very intriguing recent experimental work that has demonstrated bandgap engineering in ternary (AlxGayIn1-x-y)2O3 ranging from 3.8 eV to 7.5 eV by adjusting the ratio of In/Ga[1] and Ga/Al.[2] We employed DFT-based cluster expansion (CE) models combined with fast stochastic optimization techniques (e.g., Wang-Landau and diffusive nested sampling) in order to efficiently search for stable and metastable configurations of (AlxGayIn1-x-y)2O3 at various lattice structures. The approach also allows for a consideration of the effect of entropy on the relative stability of ternary TCOs. Statistical learning/compressed sensing is being used to efficiently identify a structure-property relationship between the targeted properties (e.g., mobilities and optical transparency) and the fundamental chemical and physical parameters that control these properties. \[1] Zhang et al., Solid State Commun, 186, 28 (2014). \pard[2] Ito et al., Jpn. J. Appl. Phys., 51, 100207 (2012); Zhang et al., Appl. Phys. Lett., 105, 162107 (2014).

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