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Pressure-induced insulator to metal transitions in potential 3D topological insulators Ag₂Se and Ag₂Te ZHAO ZHAO, SHIBING WANG, Stanford University, ARTEM OGANOV, State University of New York at Stony Brook, PENGCHENG CHEN, Tsinghua University, HAIJUN ZHANG, Stanford University, ZHENXIAN LIU, National Synchrotron Light Source, Brookhaven National Laboratory, WENDY MAO, Stanford University — Silver chalcogenides Ag_2Se and Ag_2Te are non-magnetic compounds exhibiting interesting physics like linear magnetoresistance and dimensionality tunable band gap. To explore their behaviors under high pressure, we performed synchrotron X-ray diffraction and infrared experiments combined with evolutionary algorithm structure predictions and *ab-initio* band structure calculations. For Ag_2Se , the unusual increase of phase I's band gap and topologically nontrivial features of its band structure support β -Ag₂Se as a potential 3D topological insulator. The bulk insulating phase I first transforms to a bulk metallic phase II with 2.4 percent volume drop, marked by the appearance of the distinctive Se(Ag1)-Ag2-Se(Ag1) triple layers stacking pattern. At higher pressure, a transition from the phase II to a completely metallic phase III was observed. And for Ag₂Te, our study shows that the bulk insulating phase I first transforms into a semi-metallic phase II with the perseverance of its topologically non-trivial nature, and then to a bulk metallic phase III. Our study highlights pressure's role in tuning the electronic structures of Ag₂Se and Ag₂Te.

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