Supporting Information

Towards the Prediction of the Transport Properties of Cluster-Based Chalcogenides?

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**Fig. S1** Environments of Ag atoms in the X-ray structure (left) and models (right).

**Fig. S2** Band structure of the model 1 of Ag$_4$Mo$_9$Se$_{11}$ computed using the mBJ functional and taking into account spin-orbit interaction.
Fig. S3 Electrical resistivity $\rho$ vs T computed for Ag$_4$Mo$_9$Se$_{11}$ models and compared with experimental measurements. The relaxation time is fitted in order that the averaged electrical conductivities resulting from measurements and BTE calculations match.
**Fig. S4** PBE and mBJ band structures of Ag$_3$Mo$_9$Se$_{11}$ models.