Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

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

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Christophe Candolfi, Bertrand Lenoir, Patrick Gougeon, Jean-François Halet and

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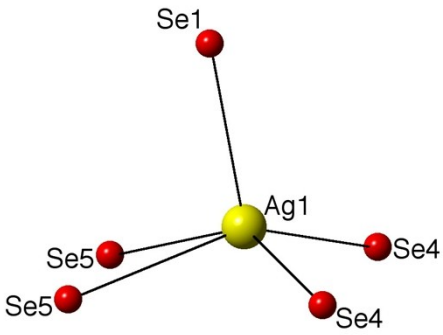
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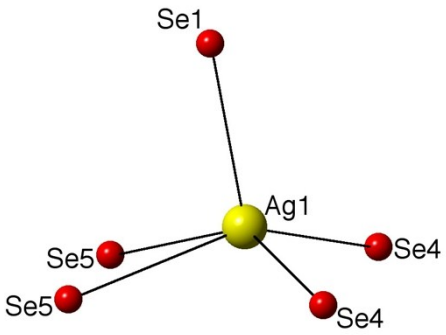
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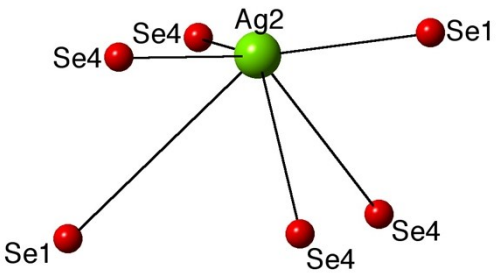
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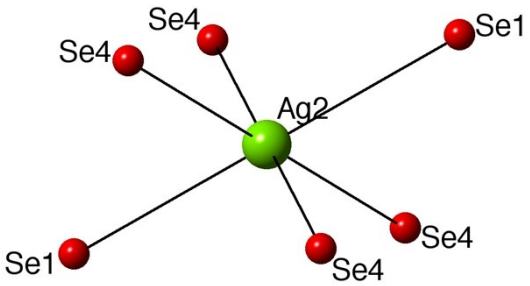
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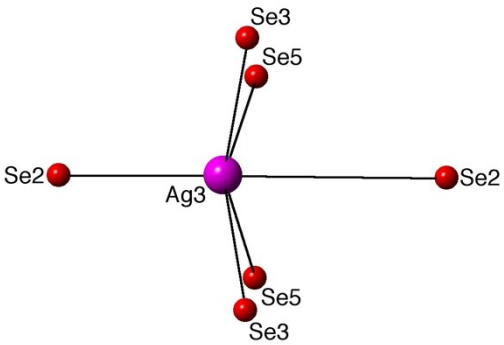
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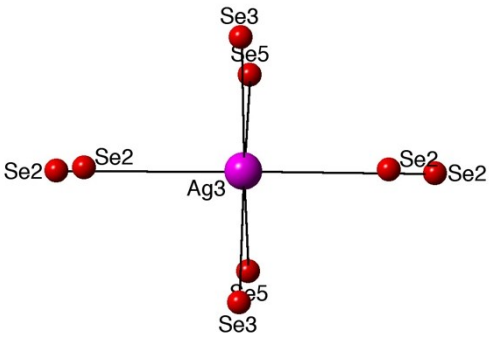
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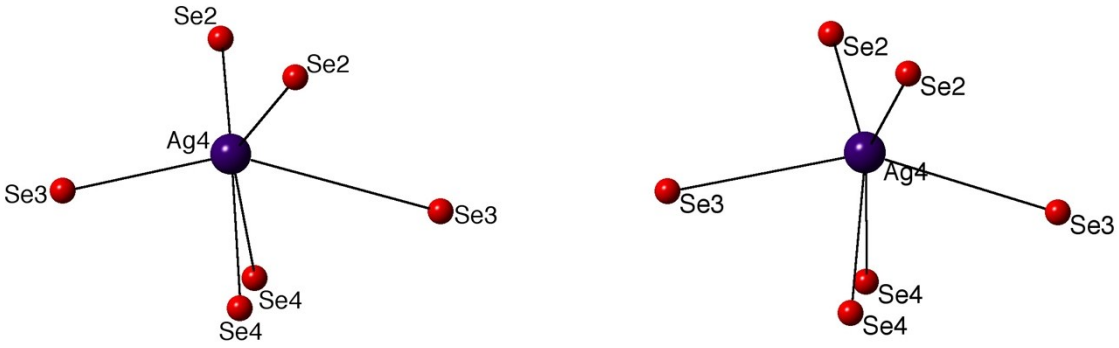

Fig. S1 Environments of Ag atoms in the X-ray structure (left) and models (right).

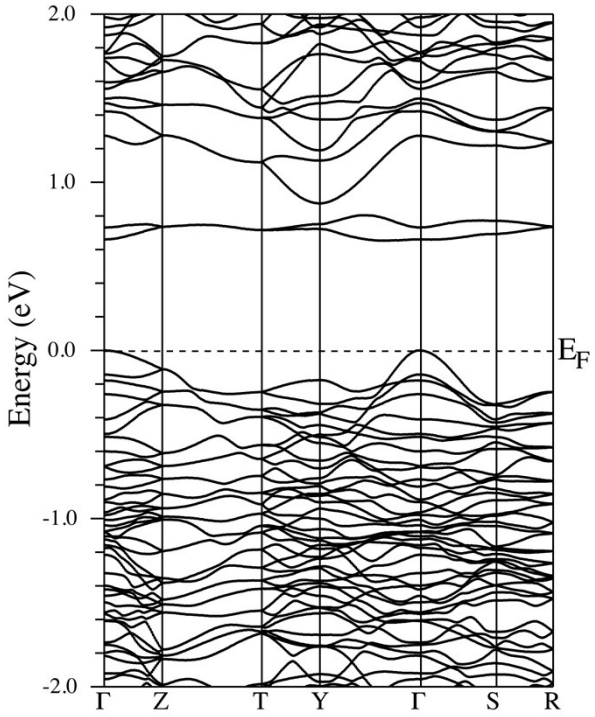

Fig. S2 Band structure of the model **1** of $Ag_4Mo_9Se_{11}$ computed using the mBJ functional and taking into account spin-orbit interaction.

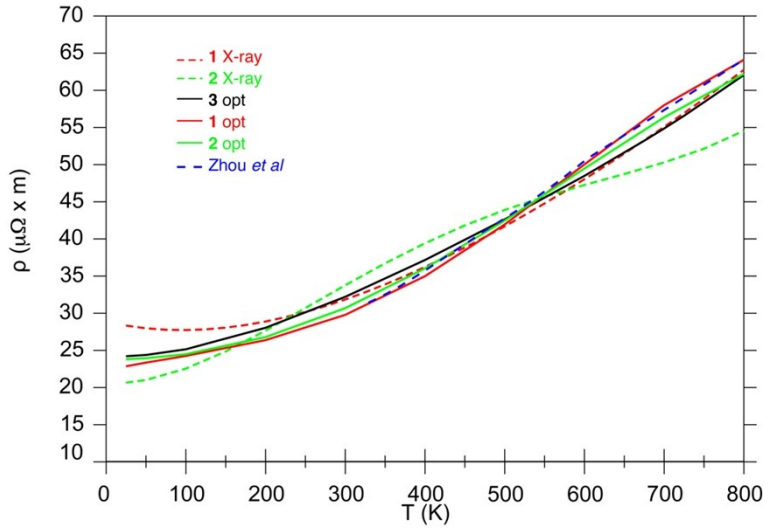

Fig. S3 Electrical resistivity ρ *vs* T computed for $Ag_4Mo_9Se_{11}$ models and compared with experimental measurements. The relaxation time is fitted in order that the averaged electrical conductivities resulting from measurements and BTE calculations match.

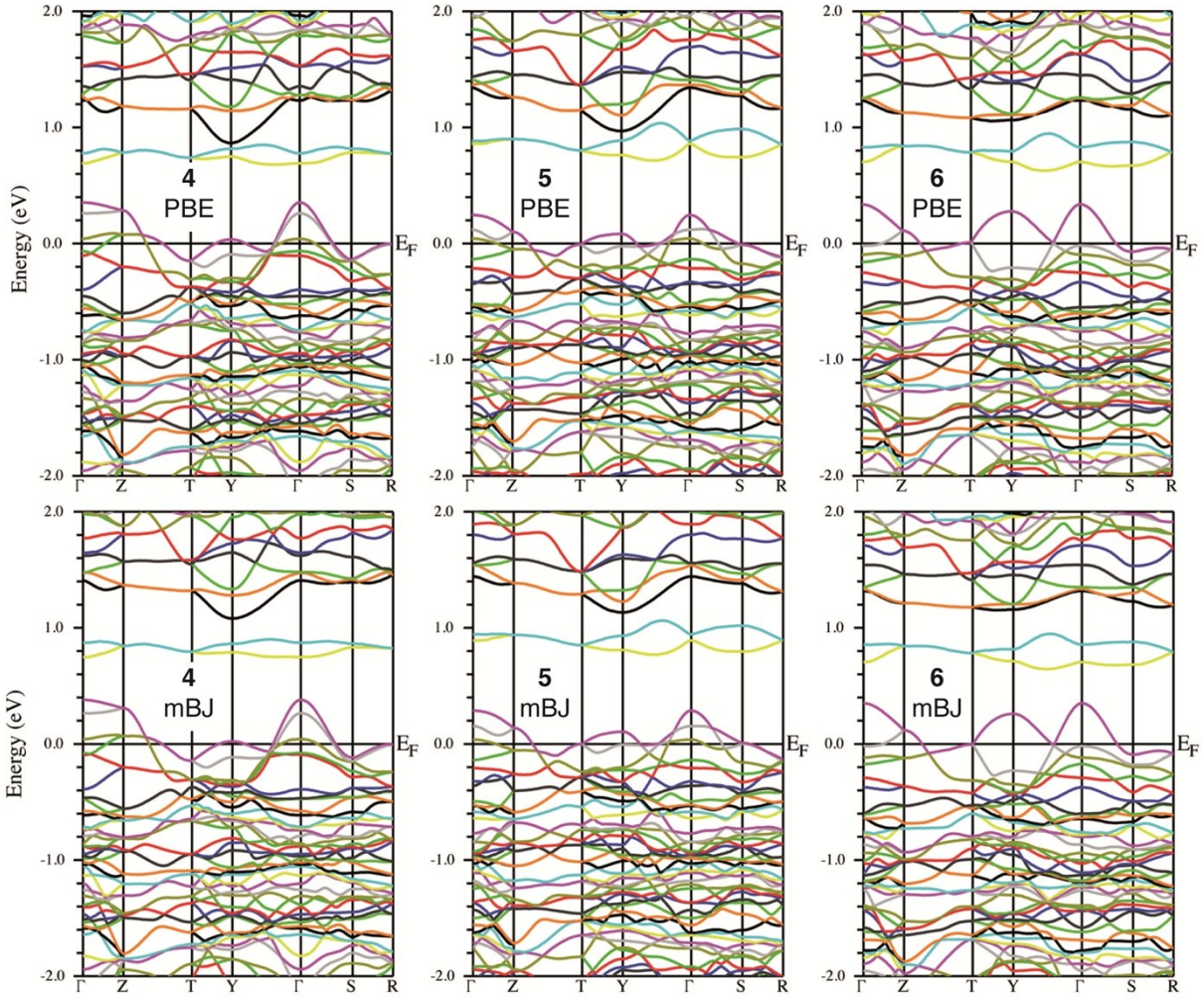

Fig. S4 PBE and mBJ band structures of $Ag_3Mo_9Se_{11}$ models.