**Use of Cluster-Based Molybdenum Chalcogenide Compounds for Thermoelectricity. Dream or Reality? A (Partial) Answer from Theory**

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Since their discovery in the earliest 70's, Chevrel-Sergent phases ($M_xMo_6X_8$; *M* = Ag, Sn, Ca, Sr, Ba, Sn, Pb, 3d elements or lanthanides; *X* = S, Se, or Te; *x* = 0−4) have been extensively studied, mainly for their superconducting properties, but also for other various applications in magnetic devices, catalysis, batteries or thermoelectricity. Later, some derivative phases were found, containing larger clusters such as $Mo_9X_{11}$ or $Mo_{30}X_{32}$ resulting from one-dimensional *trans*-face sharing of $Mo_6$ octahedra. Some of them, such as $Ag_xMo_9Se_{11}$ (*x* = 3.6 – 3.8), show outstandingly low lattice thermal conductivity, giving rise to promising thermoelectric properties. With these results in mind, electronic structure and electronic transport DFT calculations coupled with machine learning were used for the design of new cluster species which could display interesting thermoelectric properties. Some results will be presented.