Thermotactical Investigations of the Electronic and Thermoelectric Properties of Metal Oxide Materials

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Background/Relevance
- Thermoelectric (TE) materials are solid state devices that could be designed using two dissimilar materials such as n-type and p-type semiconductors. They are designed to convert thermal energy from a temperature gradient into electrical energy and visa versa.
- Oxide materials are promising materials for TE applications due to their low cost, abundance and stability against decomposition at high temperatures.

Innovation
- Using metal oxide materials in thermoelectric generators.

Key Results
- Electronic and thermoelectric properties of Zn$_x$Cd$_{1-x}$O (x = 0.125, 0.25, 0.375, 0.5, 0.625, 0.75, 0.875, and 1) alloys are investigated.
- Using the GGA-PBE functional, ZnO exhibits direct band gap of 0.731 eV and CdO presents negative and indirect band gap of -0.501 eV, while using GGA-mbj, the band gap values were improved to reach 2.670 eV for ZnO and 1.19 eV for CdO.

Approach
- The density functional theory method is used to calculate the structural and electronic properties of the ZnO and CdO pure and alloyed oxides.
- The semi-classical Boltzmann transport theory is used to calculate the thermoelectric properties that include seebeck coefficient, electrical conductivity, and electronic thermal conductivity of the materials.

Conclusions
- The metal oxide materials could be good semiconductor materials for thermoelectric devices because they have high Seebeck coefficient and a high thermal stability.
- The band gaps of Zn$_x$Cd$_{1-x}$O ternary alloys are improved using GGA-mbj hybrid functional as compared to the GGA-PBE functional.

Future Work
- Phonon calculation to investigate stability of structure.
- Calculating lattice thermal conductivity.
- Calculating figure of merit.