Contribution ID: **28** Type: **Poster Presentation**

First-Principles Study of $ZrCo_2Y/ZrCoY$ (Y=Sb, Bi, As)Interface for Thermoelectric Applications

\begin{abstract}
Half-Heusler alloys such as ZrCoSb, ZrCoBi, and ZrCoAs are promising thermoelectric materials for recovering waste heat because of their favorable electronic and thermal properties\cite{reference1,reference2}. However, achieving low-resistance electrical contact at the hot interface between half-Heusler materials and metal electrodes remains a significant challenge. Recent experimental studies indicate that a coherent interface can form between full-Heusler and half-Heusler compounds by diffusion of transition metal atoms into the vacant sublattice of the half-Heusler structure\cite{reference3}.

In this study, we employ first-principles calculations to investigate the structural and electronic properties of the $ZrCo_2Y/ZrCoY$ interface. Our results reveal that this interface exhibits low contact resistivity and nearly ohmic behavior at various temperatures and doping levels. The stability and favorable electronic characteristics of these interfaces suggest that full-Heusler compounds could serve as efficient electrical contacts for half-Heusler thermoelectric materials, enhancing the performance of thermoelectric generators.
\end{abstract}
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\bibitem{reference1} Allan, L., Mulwa, W. M., Mwabora, J. M., Musembi, R. J., Mapasha, R. E. \textbf{9}, 8 (2023).
\bibitem{reference2} Allan, L., Mapasha, R. E., Mulwa, W. M., Mwabora, J. M., Musembi, R. J. . \textbf{22} 100558(2024).

\bibitem{reference3} Spataru, C. D., He, Y., Léonard, F. \textbf{7}, 1 (2019).

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