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The Effect of Binding Groups on the Seebeck Coefficient of Phenyl Derivative Molecular Junctions[1] WILLIAM CHANG, UC Berkeley, CHENGKANG MAI, UC Santa Barbara, MICHELE KOTIUGA, JEFFREY URBAN, JEFFREY NEATON, Lawrence Berkeley National Lab, GUI BAZAN, UC Santa Barbara, RACHEL SEGALMAN, UC Berkeley — Thermoelectrics currently suffer from low efficiencies due to inverse coupling of the Seebeck coefficient and electrical conductivity, limiting the power factor. Decoupling of these two physical properties has previously been demonstrated in molecular junctions. Using an STM break junction measurement technique, we demonstrate the effect that the direct binding group Au-C has on the Seebeck coefficient. Phenyl derivative molecules with an Au-C direct binding group show a significantly lower Seebeck coefficient than molecules with an Au-S binding group. This lower Seebeck coefficient is explained by theoretical calculations as a broadening in the transmission function due to the direct bonding group. This demonstrates the importance of the metal-molecule interface and binding group selection in tuning the transmission function, and the resultant conductance and Seebeck coefficient. This result will lend further insight in rational design for molecules with higher power factors.

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