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Modulation of thermopower in heater integrated field-effect molecular devices YOUNGSANG KIM, WONHO JEONG, KYEONGTAE KIM, WOOCHUL LEE, PRAMOD REDDY, Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI, USA — Study of thermopower in molecular junctions is of great importance for understanding charge transport mechanisms as well as for making efficient energy conversion devices. In order to achieve a large thermoelectric efficiency (figure of merit, ZT), it is crucial to simultaneously increase the electrical conductance and Seebeck coefficient of junctions. The electrical conductance of molecular junctions is directly proportional to the transmission ($T(E)$) at the Fermi level (E_F), while the Seebeck coefficient is proportional to the energy derivative of $T(E)$ at E_F. In this study, we successfully fabricated electromigrated break junction with integrated heater devices to establish temperature differentials across molecular junctions and study the possibility of tuning the electronic structure to simultaneously increase $T(E)$ and its energy derivative at E_F. Further, using this platform, we studied the thermopower and the I-V characteristics of molecular junctions while modulating the electronic structure using a gate electrode. Our results unambiguously show that the thermopower and the electrical conductance of molecular junctions can be simultaneously enhanced by tuning the electronic structure. These results could pave the way for both understanding energy conversion at the molecular scale and the development of novel thermoelectric devices.

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