Thermoelectric Measurements of Self-Assembled Monolayer of Multinuclear Ruthenium Alkynyl Complexes

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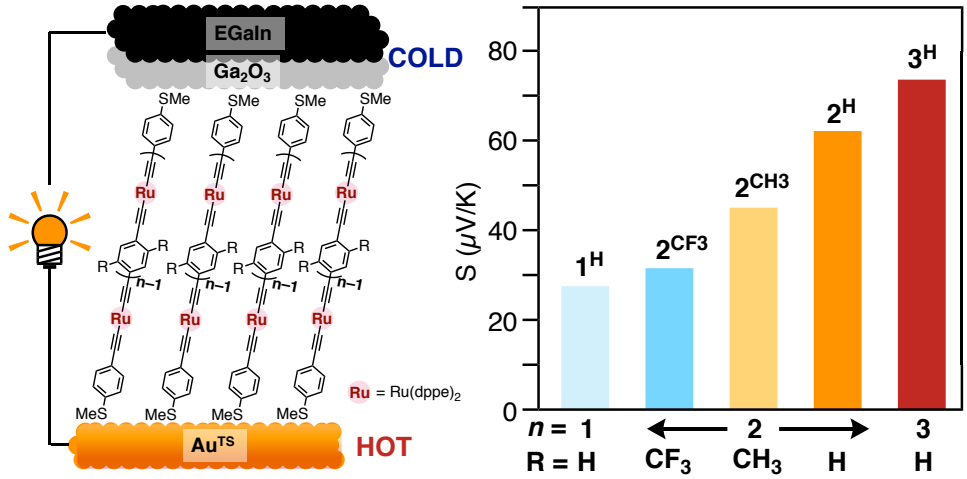
Molecules with high Seebeck coefficients (*S*) have potential applications in thermoelectric materials. However, their *S* values at single-molecule and self-assembled monolayer levels are low partly due to large energy gaps ($E–E_F$) between molecular frontier orbital energy and Fermi energy of the electrodes. We have recently reported highly conducting organometallic molecules with electron-rich ruthenium tetraphosphine fragments in molecular junction.[1] The theoretical study suggests that their small energy gaps ($E–E_F$), which may lead to a large Seebeck coefficient. In this study, we report the Seebeck coefficient of multinuclear ruthenium complexes bridged by *p*-diethynylbenzene-diyl linkers and examine their thermoelectric properties.[2]

Thermoelectric measurements for mono-, di- and tri-ruthenium complexes $\mathbf{1^R}$-$\mathbf{3^R}$ (R = H, CF_3, OMe) were conducted using the Au-molecule-EGaIn/Ga_2O_3 system.[3] Upon heating the gold electrode, the *S* values increased with the number of metal fragments, and the trinuclear complex showed a value exceeding 70 μV/K, which is the highest *S* value obtained by SAM junction reported so far. Theoretical calculations and cyclic voltammograms indicate that the high Seebeck coefficient is caused by the high-lying HOMO, which destabilizes as the number of metal fragments increases. We also examined substituents effect for the dinuclear complexes ($\mathbf{2^R}$).



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