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Computational-enabled Design and Electrostatic Doping in 2D Materials for Quantum and Neuromorphic Information Processing[1]

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van der Waals (vdW) materials designed with 2D materials exhibit one of the broadest sets of novel properties that are highly desirable for enabling heterogeneous device concepts such as neuromorphic and quantum computing. Their flexible electronic structures facilitate efficient control and tuning of both the carrier dynamics and charge injection with either chemical or electrical doping. In this talk, I will demonstrate some of our recent findings unveiling a unique material design concept at the interface of molecular electronics and 2D-based vdW materials. We achieved efficient electrostatic doping in transition metal dichalcogenide based homostructure of HfS_2 by electrochemical intercalation of organometallic molecular species of the metallocene family – MCP_2 (M = Cr, Co, Fe, Ni, etc.). The molecular intercalants behave as pseudo-alkali atoms transferring electrons to the host material. The designed HfS_2-$CrCP_2$ hybrid material revealed multi-switching capabilities with ultrahigh dynamical control of over 400 folds (i.e., from 1.8 μ/cm to 741 μ/cm) of the cross-planar electrical conductivity. Our findings show a promising route to create an organic/inorganic interface that tunes and tailor the properties of host materials for novel device applications such as quantum and neuromorphic information processing. I will discuss a proposed machine-learning-enabled design approach to speed up the material design process – identifying both the host material and promising molecular guest species.

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