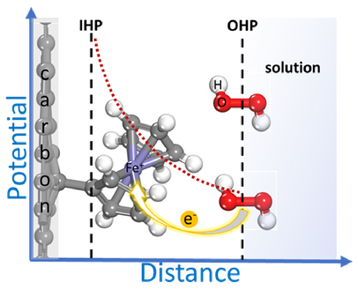
New Energy Solutions with Computational Materials Chemistry

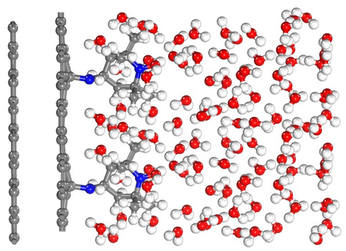
Electrochemical Catalysis

$$i\frac{\partial}{\partial t}\Phi = \hat{H}\Phi$$

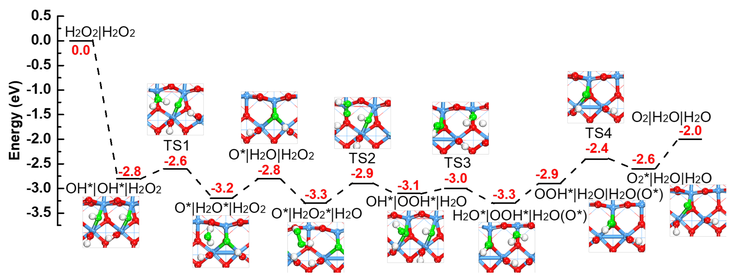
$$\hat{H} = \underbrace{-\sum_n \frac{\hbar^2}{2M}\nabla_n^2}_{\hat{T}_R} \underbrace{-\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2}_{\hat{T}_r} \text{ Kinetic terms}$$
$$+ \underbrace{\frac{1}{4\pi\epsilon_0}\frac{1}{2}\sum_{n\neq m}\frac{Z_n Z_m e^2}{|\boldsymbol{R}_n - \boldsymbol{R}_m|}}_{\hat{V}_R} + \underbrace{\frac{1}{4\pi\epsilon_0}\frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}}_{\hat{V}_r}$$
$$+ \underbrace{-\frac{1}{4\pi\epsilon_0}\sum_{i,n}\frac{Z_n e^2}{|\boldsymbol{r}_i - \boldsymbol{R}_n|}}_{\hat{V}_{r,R}} \text{ Potential terms}$$

Density Functional Theory (DFT): Good balance between accuracy and computational cost

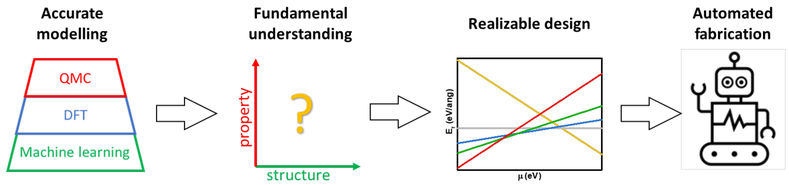




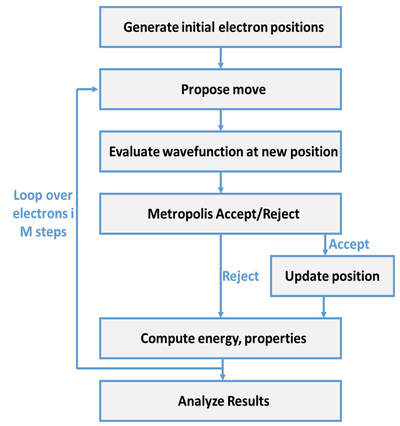
Understanding complex electrochemical interfaces and mechanisms of electron transfer and catalytic reactions



Developing closed-loop computational frameworks for functional materials



Neuromorphic Computing

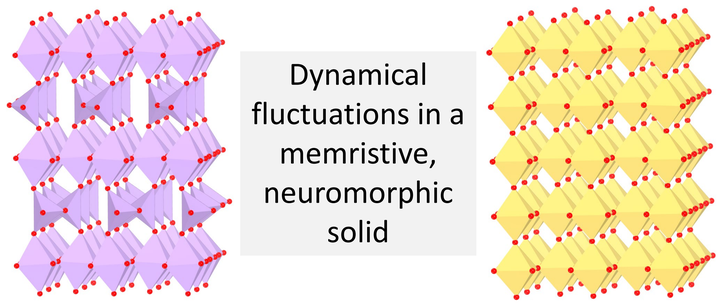


Quantum Monte Carlo (QMC): Accurate description of complex electronic structures

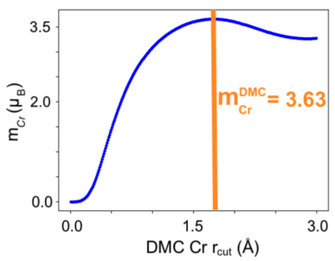
Diffusion Monte Carlo (DMC)

$$\lim_{t\to\infty} e^{-t(\hat{H}-E_0)}\Psi_T = \Psi_{0,\mathrm{FN}} \geq 0,$$
$$\Psi_T = e^{J_1+J_2}\Phi_T.$$

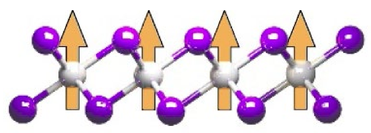
Providing accurate predictions of structural, electronic, and magnetic properties of strongly correlated quantum materials



Dynamical fluctuations in a memristive, neuromorphic solid



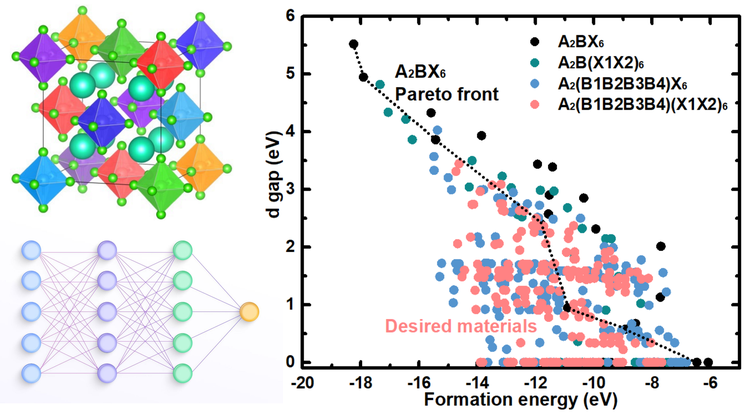
2D magnet CrI_3



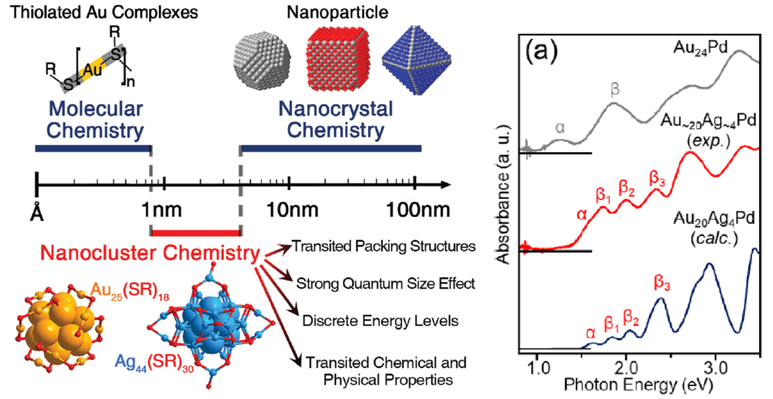
Light Harvesting

Informatics and AI: Feasibly screening wide chemical and structural spaces

Designing and discovering novel materials such as high entropy materials to go beyond the Pareto front



Revealing optical properties of ligand protected atomically precise metal nanoclusters



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