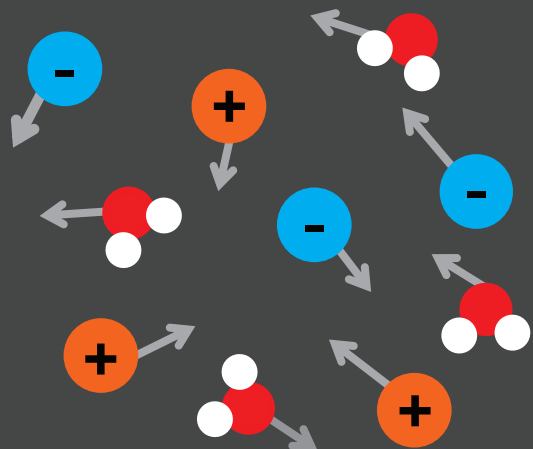


## Multi-scale Modeling

Statistical mechanics and quantum mechanics

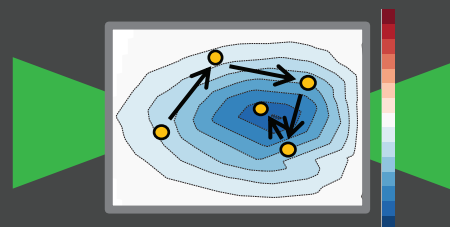
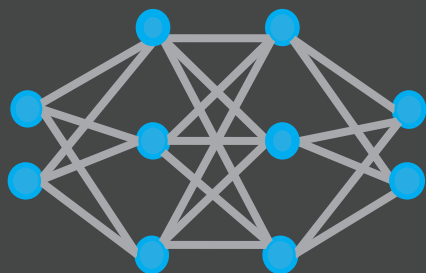


## MOLECULAR DESIGN FOR WATER, ENERGY, AND SUSTAINABILITY



## Machine-Learning

Potential energy surface (PES) development, structure-property relationships, generative design



## Chemical Informatics

Molecular fingerprinting and high throughput screening

