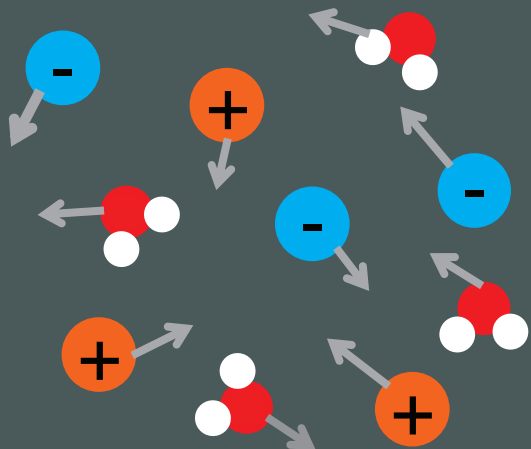


Multi-scale Modeling

Statistical mechanics and quantum mechanics

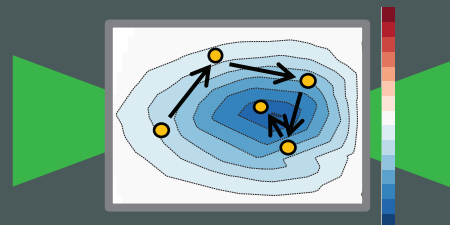
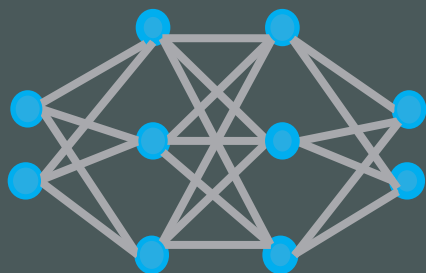


MOLECULAR DESIGN FOR WATER AND ENERGY SYSTEMS



Machine-Learning

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



Chemical Informatics

Molecular fingerprinting and high throughput screening

