

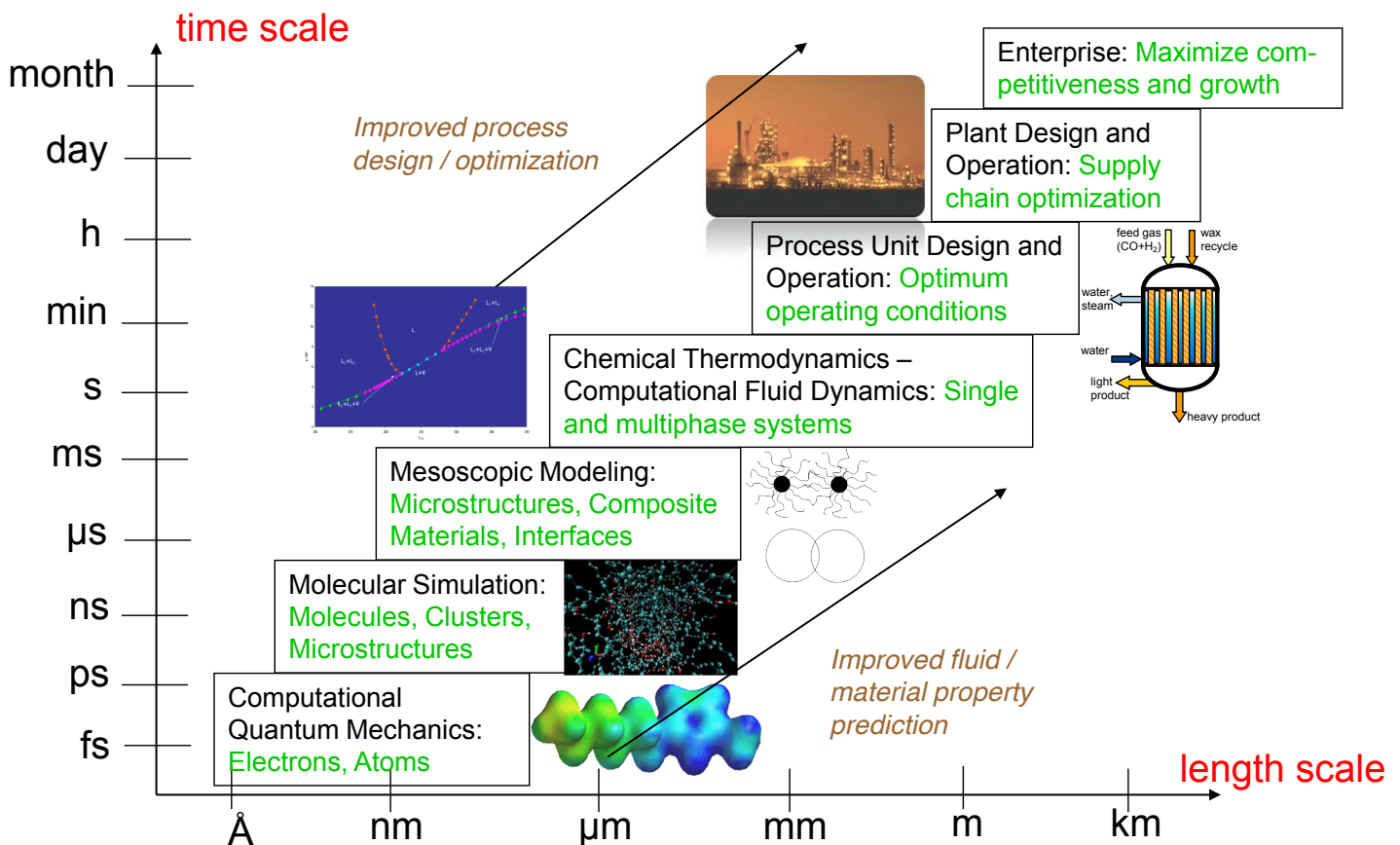


Molecular Thermodynamics: A Powerful Tool for Chemical Process and Product Design

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Hierarchical multi-scale process modeling



The accurate knowledge of physical properties and phase equilibria of complex fluids is a critical factor towards the design and optimization of chemical processes and novel products. Thermodynamic models with strong physical basis provide the means to understand and quantify interactions and phenomena at the molecular and mesoscopic level and eventually predict macroscopic properties of interest. The unprecedented increase of computing power at relatively low price in recent decades has allowed the development of predictive methods that span the entire range of length and time scales, from sub-atomic quantum mechanical calculations up to macroscopic equations of state. In this presentation, we will discuss molecular simulation methods that are used widely and we will present representative examples from our own research with direct applications to oil & gas and chemical industry, and for carbon capture and sequestration applications. In addition, we will highlight work on the development of a statistical mechanics-based equation of state for the prediction of complex mixture phase equilibria. In all cases, comparison against experimental data will be shown.