CHEMISTRY & BIOCHEMISTRY COLLOQUIUM: Importance of Electrostatics and the Role of Interfaces for Chemical Transformations

Teresa Head-Gordon
Professor of Chemistry
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Date:
9/9/2022

Time:
1:30 PM-2:50 PM

Location:
COB 267

About The Speaker:

Teresa Lyn Head-Gordon (*née* **Teresa Lyn Gordon**) is an American chemist and the Chancellor's Professor of Chemistry, Bioengineering, and Chemical and Biomolecular Engineering at the University of California, Berkeley.[4] She is also a faculty scientist in the Chemical Sciences Division at the Lawrence Berkeley National Laboratory and a fellow of both the American Institute for Medical and Biological Engineering (AIMBE) and the American Chemical Society (ACS).[5]

For more detailed information on the speaker plesae visit:
https://en.wikipedia.org/wiki/Teresa_Head-Gordon

Abstract:

Chemical transformations rarely occur in a single homogeneous aqueous phase, but instead occur in niches, crevices, and impurity sites at confining interfaces between two or more phases of gases, liquids or solids. Fundamentally, interfaces can alter solvent and solution compositions and phases to reformulate the transition states and pathways of chemical reactions and underlying transport mechanisms. Computational modeling of these systems thereby requires an accurate description of molecular interactions, especially electrostatics, of these complex system. I will present results on how electric fields have been used to computationally optimize biocatalytic performance of a synthetic enzyme, and how they could be used as a unifying descriptor for catalytic design across a range of homogeneous and heterogeneous catalysts including recent hypotheses around microdroplet chemistry. I will also discuss some methodological advances from accurate many-body force fields under non-reactive approximations in classical molecular dynamics, to reactive force fields to describe chemical reactions where charge flow is an essential process.

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