UNIVERSITÄT DUISBURG ESSEN | PHYSIK E=

Physikalisches Kolloquium

Mittwoch, 08.05.2024
13:00 Uhr
MC 122 und Zoom

https://uni-due.zoom-x.de/j/64228670246?pwd=RjVQeFNIUkRKRkpiNVpKYXhJaFNLdz09

Enhanced Chemical Reactivity on the Surface of Water

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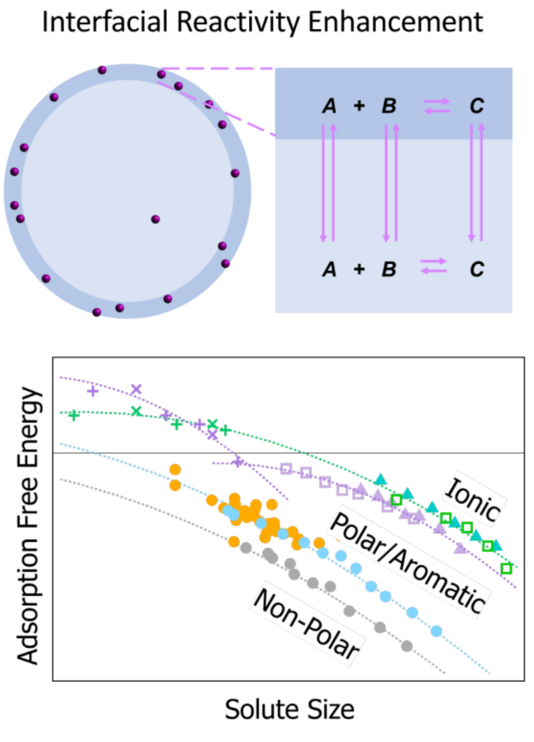

The enhancements of chemical reaction rates and yields at an air-water interface are quantified using a combined theoretical and experimental strategy.[1] The theoretical results imply that interfacial reactivity enhancement is driven primarily by the surface activity of the product (or activated complex), while reactants have a smaller indirect influence on reactivity due to compensating interfacial concentration and reaction free energy changes. Experimental adsorption free energies and critical micelle concentration correlations are used to quantify adsorption free energies and interfacial reactivities as a function of solute size, polarity, and change. The results are illustrated using predictions of interfacial changes in S_N2 reaction rates and fatty acid pK_a on water micro-droplets.

(1) Dor Ben-Amotz, J Chem Phys 160 084704 (2024).