The field of interface science covers the physicochemical properties and behavior at the boundary between two phases. It is an integral part of a vast range of research topics, such as adsorption, catalysis, electrochemistry, biochemistry, and geochemistry. It is an extensively studied field and covers the chemistry of colloids, metals, semiconductors, micelles and surfactants, cells and proteins, soils and minerals, aerosols, and more.

Adsorption involves the attachment of chemical species (adsorbates) at an interface (adsorbent), often solid-liquid or solid-air. It is a complex process to study and understand since not only the adsorbate-adsorbent interactions have to be taken into account, but also the interactions between the adsorbates, ions, solvent molecules, and the surface. One potential field of application for adsorption is odor capture. Effective odor capture could improve the living standards of hundreds of millions of people with urinary incontinence worldwide.

This thesis work investigates the influence of ions on the surface properties of silica nanoparticles and crystalline nanocellulose. We could establish a distinct co-ion effect on the surface charge of silica due to ion pairing - an effect that is enhanced near charged interfaces. We discovered that ion and surface hydration plays a crucial role when interacting with each other, and this was observed as a trend reversal in the counter-ion affinity for the sulfate groups on the nanocellulose surface at alkaline pH.

The adsorption of the odorant p-cresol on carbon-based materials in synthetic urine was studied through experimental and computational means. Structure-making ions (Na^+, Mg^{2+}, Ca^{2+}) and urea lead to enhanced p-cresol adsorption on the most hydrophobic activated carbon, owing to the salting out effect. The simulations show that the pristine graphene sheet interacts the strongest with p-cresol in synthetic urine. As the sheet obtains oxygen functional groups and surface charge, counter-ion accumulation near the interface repels the p-cresol molecules.

ISBN: 978-91-8009-917-2 (TRYCK)
ISBN: 978-91-8009-918-9 (PDF)

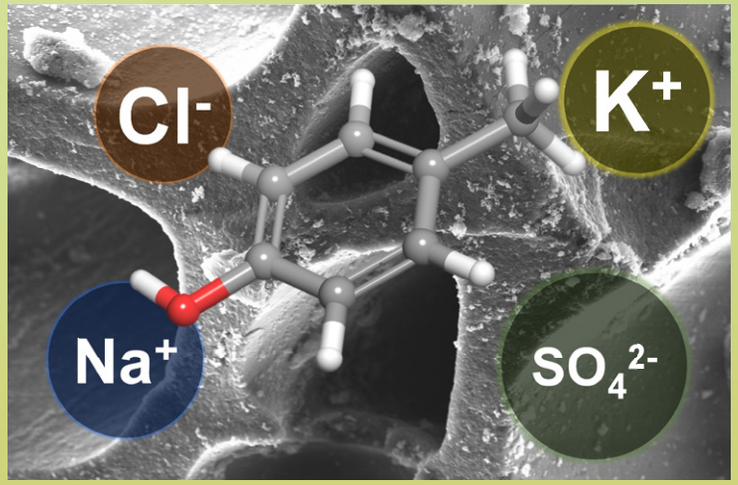
Ph.D. thesis

On the Interactions of Ions and Odor Molecules with Nanomaterials in Water and Synthetic Urine | Isabelle Simonsson 2022

PH.D. THESIS

On the Interactions of Ions and Odor Molecules with Nanomaterials in Water and Synthetic Urine

Isabelle Simonsson



DEPARTMENT OF CHEMISTRY
AND MOLECULAR BIOLOGY

UNIVERSITY OF
GOTHENBURG