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Accurate Molecular Models of Natural and Environmental Materials

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The transition to net-zero emissions and delivering water security across the globe are key challenges that necessitate innovative material solutions. In this talk, I will discuss molecular simulations and how they can aid the development of more efficient and cleaner technologies – from water filtration, and pollution remediation, to carbon storage. I will detail the contributions of my research group to these challenges by delivering accurate molecular models of clay minerals and biochar materials, both characterised by high surface areas and tuneable properties for selective pollutant adsorption.

Our recent work has focused on developing realistic molecular models of biochars, constructed from experimental data.[1-3] These models are pivotal for simulating and understanding the molecular interactions that govern biochar's ability to capture CO2, purify water, and enhance soil nutrient retention. For instance, our findings highlight the critical role of feedstock and production conditions in defining biochar's functional properties, highlighting the key elements for the successful removal of pollutants like manganese from water bodies.

Parallelly, our work with clays and layered minerals has led to the development of rigorous computational protocols. These protocols accurately simulate interactions with various molecules under diverse environmental conditions, including scenarios reminiscent of early Earth.[4-6] The recent development of ClayCode, a computational tool for setting up realistic clay mineral structures, has been instrumental in bridging the gap between theoretical models and environmental applicability.[7]

Through this talk, I aim to demonstrate how molecular simulations can provide detailed insights into the physicochemical interactions that underpin critical environmental processes. We always ensure our codes, training materials, datasets and models are open to the community via our GitHub page https://github.com/Erastova-group. Through our work we hope to foster interdisciplinary collaboration, and we can drive the material innovations necessary to achieve global and local environmental challenges.

References:
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