

Defence announcement

Public Defence on 12th December 2023

Modelling self-assembly and adsorption in bio-oils

Title of the doctoral thesis	Computational modelling of adsorption and aggregation in bio oils at multiple length scales
Content of the doctoral thesis	<p>Surfactants, such as lipids, spontaneously self-assemble in bio oils to form diverse structures. These self-assembled structures, together with interaction of the surfactant at oil – solid interfaces, affect both the rheological properties and chemical reactivity of the oil, which are crucial for down-stream processing of the oil.</p> <p>In this doctoral thesis, the self-assembly and adsorption of lipids and other typical bio oil minority components is modelled at multiple length and time scales. Atomistic molecular dynamics simulations, mesoscale dissipative particle dynamics simulations, and equilibrium state thermodynamic modelling are used in tandem to investigate the effects of nanometer scale phenomena, such as hydrogen bonding, electrostatics, and hydration, as well as, to simulate large scale aggregate structures and competitive adsorption phenomena. Importantly, the results and presented models give new perspective for interpreting experimental isotherm data, and allow tuning of surface structures based on lipid head group structure, oil water content, and surface hydrophilicity.</p> <p>The results provide additional insight into self-assembly and adsorption in both bio oils and apolar solvents in general. The sensitivity and tunability of the examined bio oil systems in terms of molecular chemistry of both the oil and adsorbent surface, and presence of additives, as well as, the diversity of adsorption mechanisms and adsorbed surface structures are of particular note for designing chemical engineering processes.</p>
Field of the doctoral thesis	Soft materials modelling
Doctoral candidate and contact information	M.Sc. (Tech.) Maisa Ilona Vuorte mais.vuorte@gmail.com
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Remote defence	https://aalto.zoom.us/j/65849665956
Place of public defence	Aalto University School of Economics, Jenny ja Antti Wihurin Rahasto lecture hall, Ekonomianaukio 1, Espoo
Opponent(s)	Professor Mark Wilson, Durham University, UK
Custos	Professor Kari Laasonen, Aalto University School of Chemical Engineering
Link to electronic thesis	https://aaltodoc.aalto.fi/handle/123456789/51
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