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Water at Interfaces: A Molecular Approach

Jordi Fraxedas

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Water, with its simple molecular structure, reveals a complex nature upon interaction with other molecules and surfaces. **Water at Interfaces: A Molecular Approach** provides a broad, multidisciplinary introduction to water at interfaces, focusing on its molecular characteristics. The book considers interfaces at different length scales from single water molecules to involvement of large numbers of water molecules, and from one-dimensional to three-dimensional interfaces. It begins with individual water molecules, describing their basic properties and the fundamental concepts that form the basis of this book.

The text explores the main interfaces involving pure and ion-free condensed (liquid and solid) water, including water vapor/liquid water, liquid/oil, and liquid/solid interfaces. It examines water molecules on ideal surfaces?well-ordered (crystalline) and defect-free?covering topics such as electronic structure using frontier orbitals and substrate-induced structuring. The book discusses the affinity of water to surfaces, hydrophobicity and hydrophilicity, emphasizing two extreme cases of affinity. It then addresses real solid surfaces where water/solid interfaces play a key role in actual working conditions, examining water purification, photocatalytic activity, corrosion and degradation, and atmospheric agents.

The final chapter deals with the interaction of water with the heterogeneous and complex surfaces of biomolecules, which can both influence the structure of the surrounding water and be modulated by the surrounding liquid. The author discusses simple to more complex biomolecules from peptides to proteins, nucleic acids, and membranes.

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