



Method to Calculate the Adsorption Free Energy of a Pollutant as Function of Temperature

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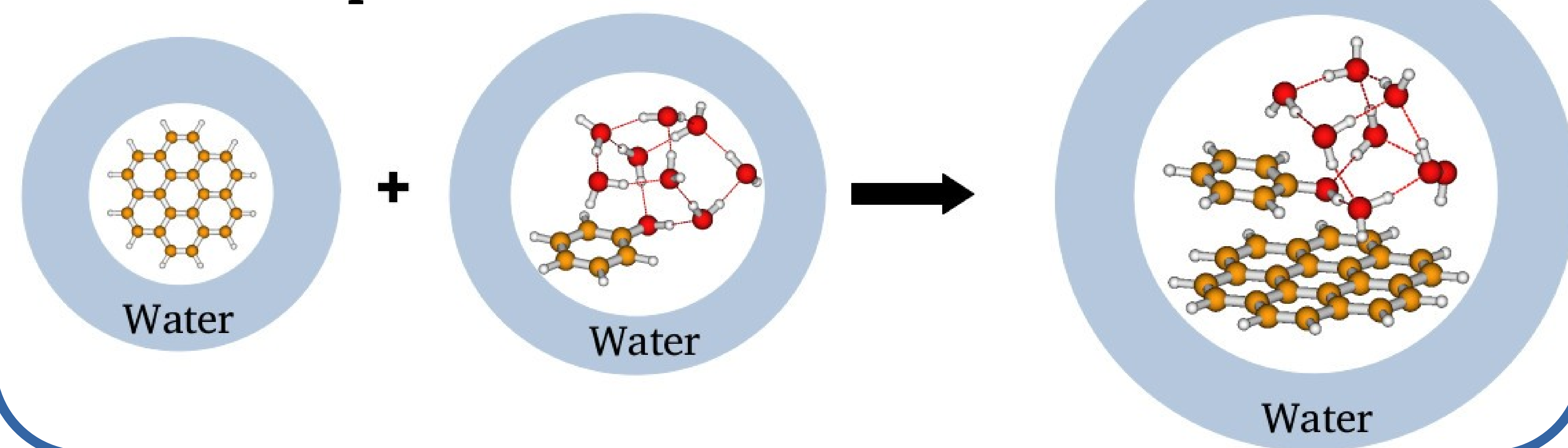
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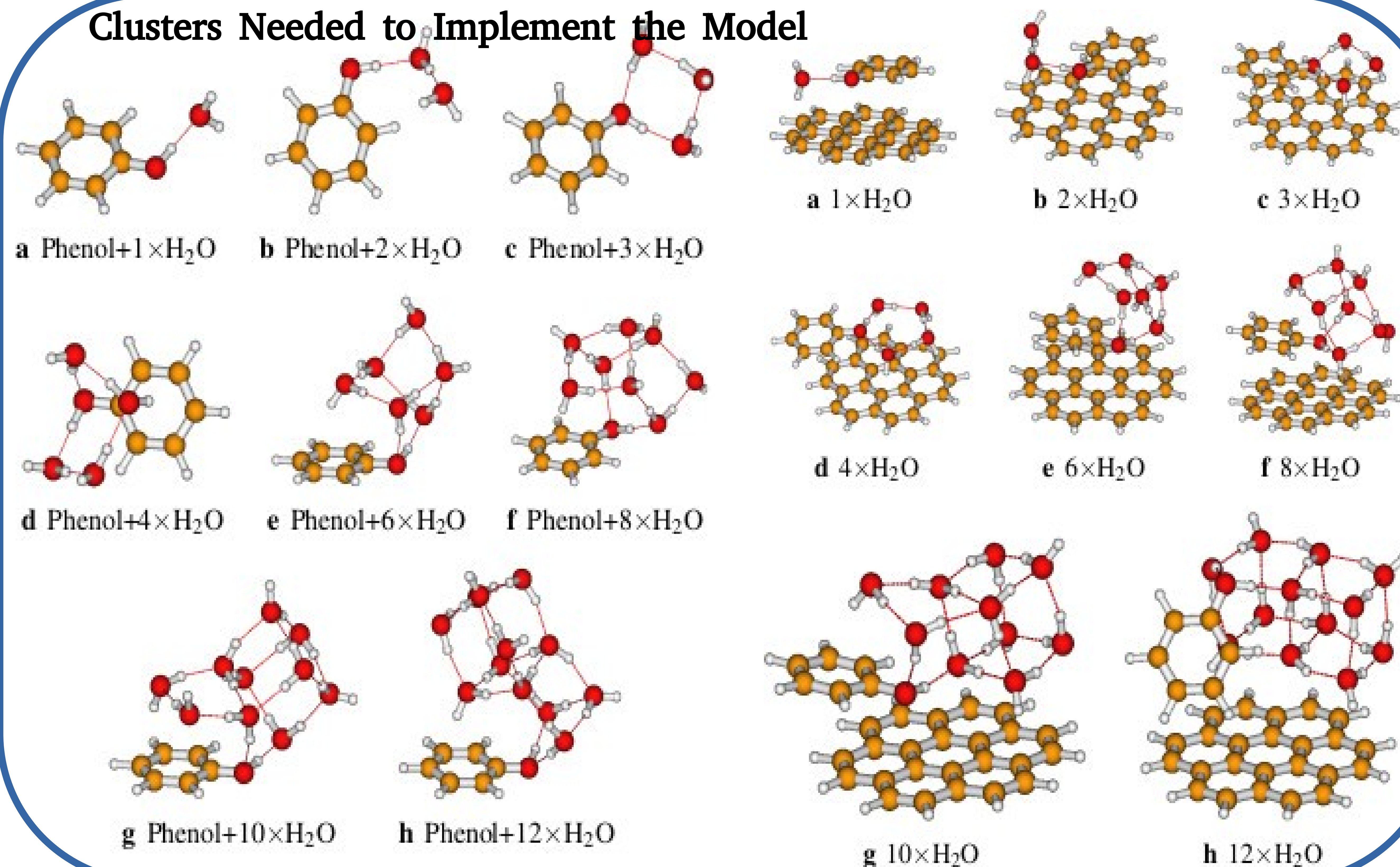
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Introduction: Molecular modeling can considerably speed up the discovery of materials with high adsorption capacity for wastewater treatment. Despite considerable efforts in computational studies, the molecular modeling of adsorption processes has several limitations in reproducing experimental conditions. Handling the environmental effects (solvent effects) and the temperature effects are part of the important limitations in the literature. In this work, we address these two limitations using the adsorption of phenol onto coronene as case study.

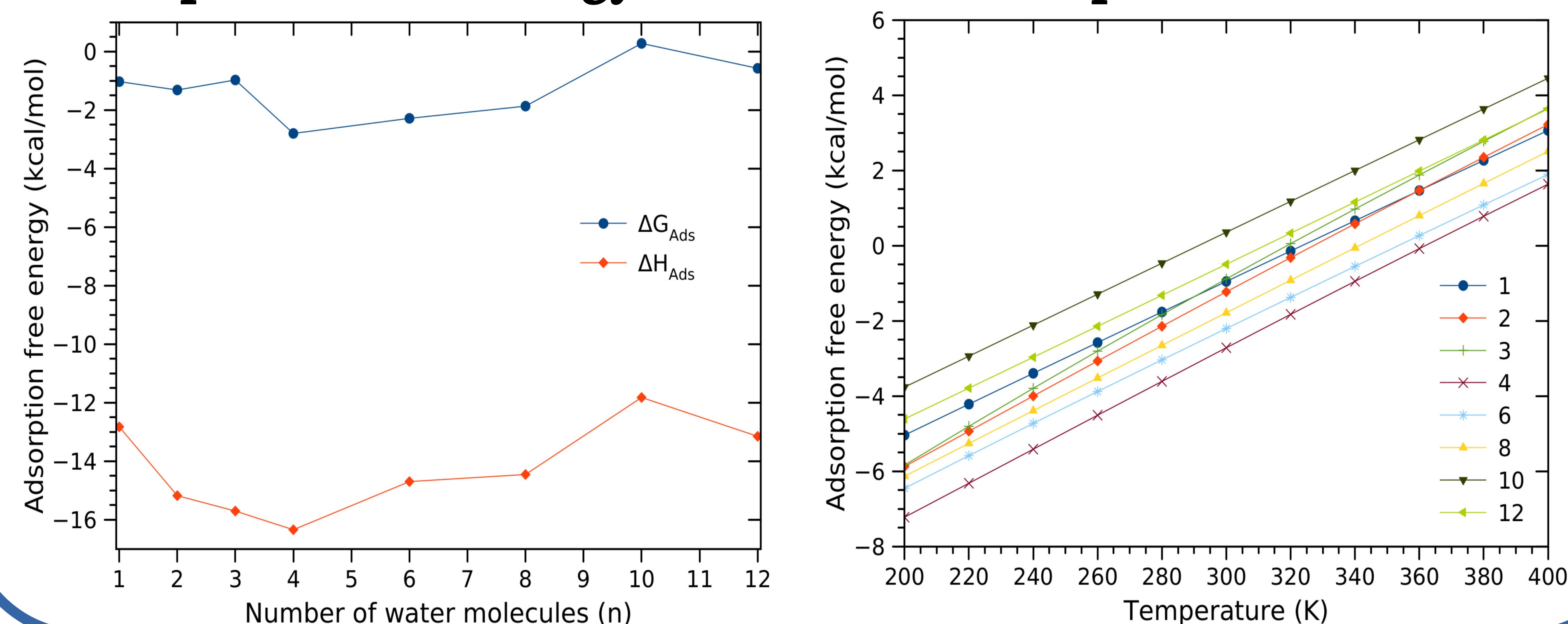
Schematic Representation of the Model



Clusters Needed to Implement the Model



Adsorption Free Energy at Different Temperature



References: A. Malloum, J. Conradie, Adsorption free energy of phenol onto coronene: Solvent and temperature effects, J. Mol. Graph. Model. 118 (2023) 108375

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