

**Title :** Investigating the Viability of Gaussian Process Regression to Produce a 1-Dimensional Free Energy Landscape of the  $Mg^{2+}$  -  $Cl^-$  Ions Association Process in an Aqueous Solution.

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## ABSTRACT

The free energy surface (FES) is crucial for identifying the relative stability of a system and can also elucidate the mechanism of chemical reactions through the minimum free energy path (MFEP). In this work, we explore the integration of Well-Tempered Metadynamics (WT-MTD) with Gaussian Process Regression (GPR) to efficiently reconstruct the free energy surface. This approach is applied to study the ion-pairing process of  $Mg^{2+}$  and  $Cl^-$  in an aqueous environment. The accuracy of the reconstructed free energy surface from Gaussian Process Regression (GPR) the results are compared with free energy profiles obtained from Umbrella Sampling (WHAM) and literature data. The reference profile is selected based on the most closely aligns with the literature results. Although applying Gaussian Process Regression (GPR) to a one-dimensional free energy surface might seem to add complexity to the Well-Tempered Metadynamics (WT-MTD) simulation, which already provide reasonable free energy estimates, this study demonstrates that Gaussian Process Regression (GPR) can accurately reconstruct the free energy surface, achieving high accuracy with relatively small training datasets.

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