

Quantifying specific ion effect through perturbed reactivity descriptors

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The mystery of ion selectivity in electrolyte solutions has puzzled scientists for centuries. The Hofmeister series observes that the selection of ions is specific, demonstrated in ion channels, metal-organic frameworks, polymers, and ionic liquids. It remains little known why nature is keen on selecting one ion over the other, despite having very similar characteristics. Previously in Gregory *et al.*, ion property was approximated through a simple empirical formula consisting of the charge and effective radius. To improve the generality and accuracy of these models, magnitudes extracted from conceptual DFT can approximate the charge and radius of an ion with or without perturbed descriptors, and using different models of charge transfer in solution. Different formulas with unperturbed and perturbed chemical potential and chemical hardness were accessed for the accuracy and generality of the modeled ion properties, such as Gibbs free energy, enthalpy, viscosity, etc. Perturbed chemical potential and chemical hardness lead to a higher quantitative agreement between the experimental and theoretical values.