



Showcasing research from Professor Nobuyuki Matubayasi's laboratory, Graduate School of Engineering Science, Osaka University, Osaka, Japan.

Free-energy decomposition of salt effects on the solubilities of small molecules and the role of excluded-volume effects

The separated contributions from cations, anions, and water in the salt effects on solvation of *n*-alcohols and *n*-alkanes are addressed by free-energy decomposition and correlation analyses over varied salt species. The direct interaction between the anion and solute is in agreement with the Setschenow coefficient in terms of the ranking of salting-in and salting-out for *n*-alkanes. The Setschenow coefficient is well correlated to the water contribution to the excluded-volume component, which corresponds further to the change in the water density upon the addition of the salt.

As featured in:



See Stefan Hervø-Hansen, Nobuyuki Matubayasi *et al.*, *Chem. Sci.*, 2024, 15, 477.