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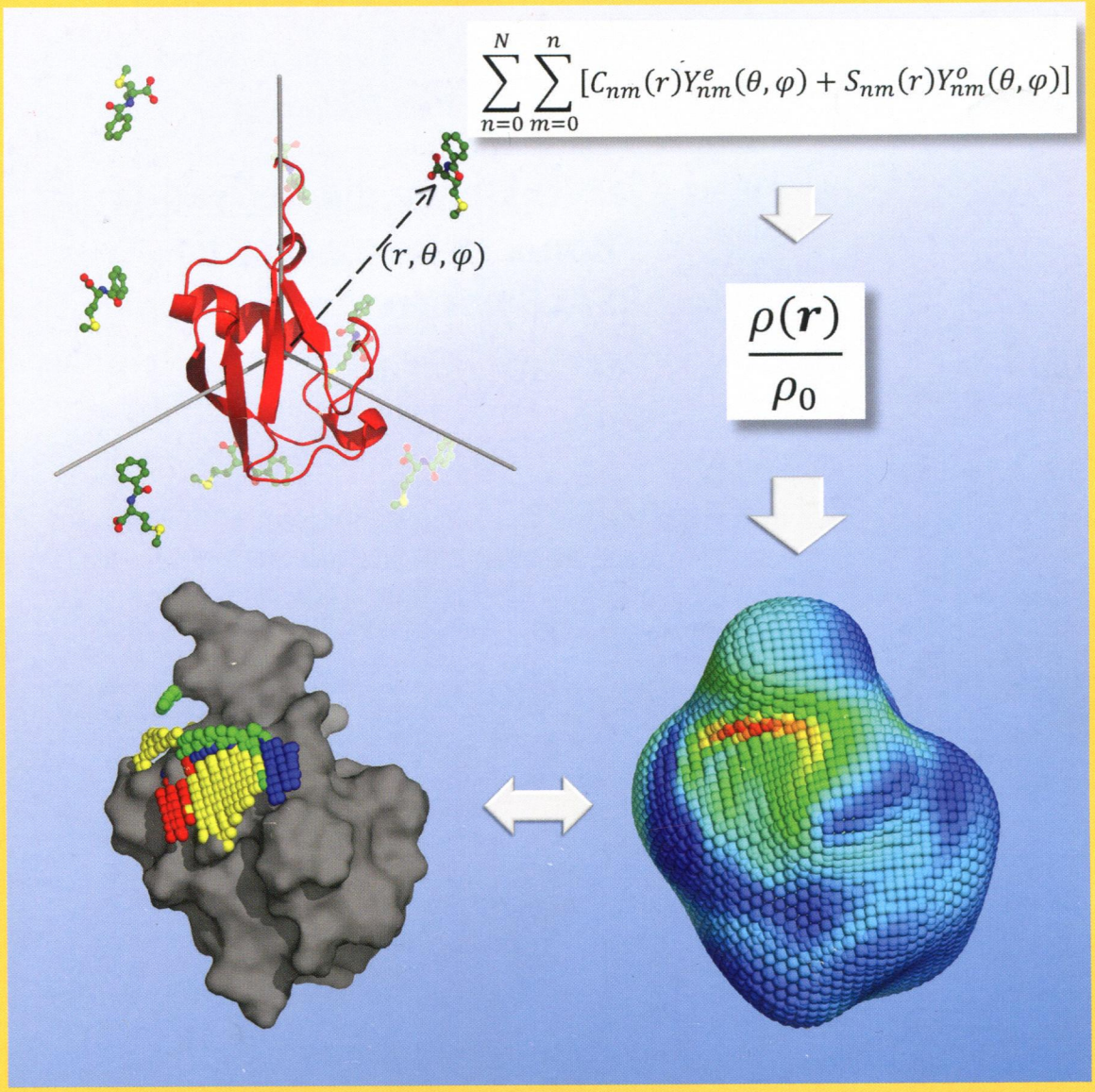

Understanding the Ligand Distribution and Binding around Proteins Using a Spherical Harmonic Expansion Approach
(see page 13066)

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER

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ON THE COVER: Parimal et al. employ a spherical harmonic expansion approach to obtain spatially resolved three-dimensional distributions of multimodal ligands around proteins from molecular dynamics simulations. Representing ligand densities using color maps on surface envelopes surrounding proteins provides an understanding of ligand binding, orientation, and synergistic interactions that may drive protein−ligand interactions. This understanding is central to modern bioseparations processes (e.g., through the design of new classes of multimodal chromatographic ligands) and in drug discovery and design. See page 13066.

Articles

Biophysical Chemistry and Biomolecules

Biomaterials, Surfactants, and Membranes

Liquids; Chemical and Dynamical Processes in Solution

Glasses, Colloids, Polymers, and Soft Matter

Additions and Corrections

13321 DOI: 10.1021/jp510693c

Correction to "Polarizable Water Models from Mixed Computational and Empirical Optimization"

Philip Tröster, Konstantin Lorenzen, Magnus Schwörer, and Paul Tavan*

Supporting Information available via online article