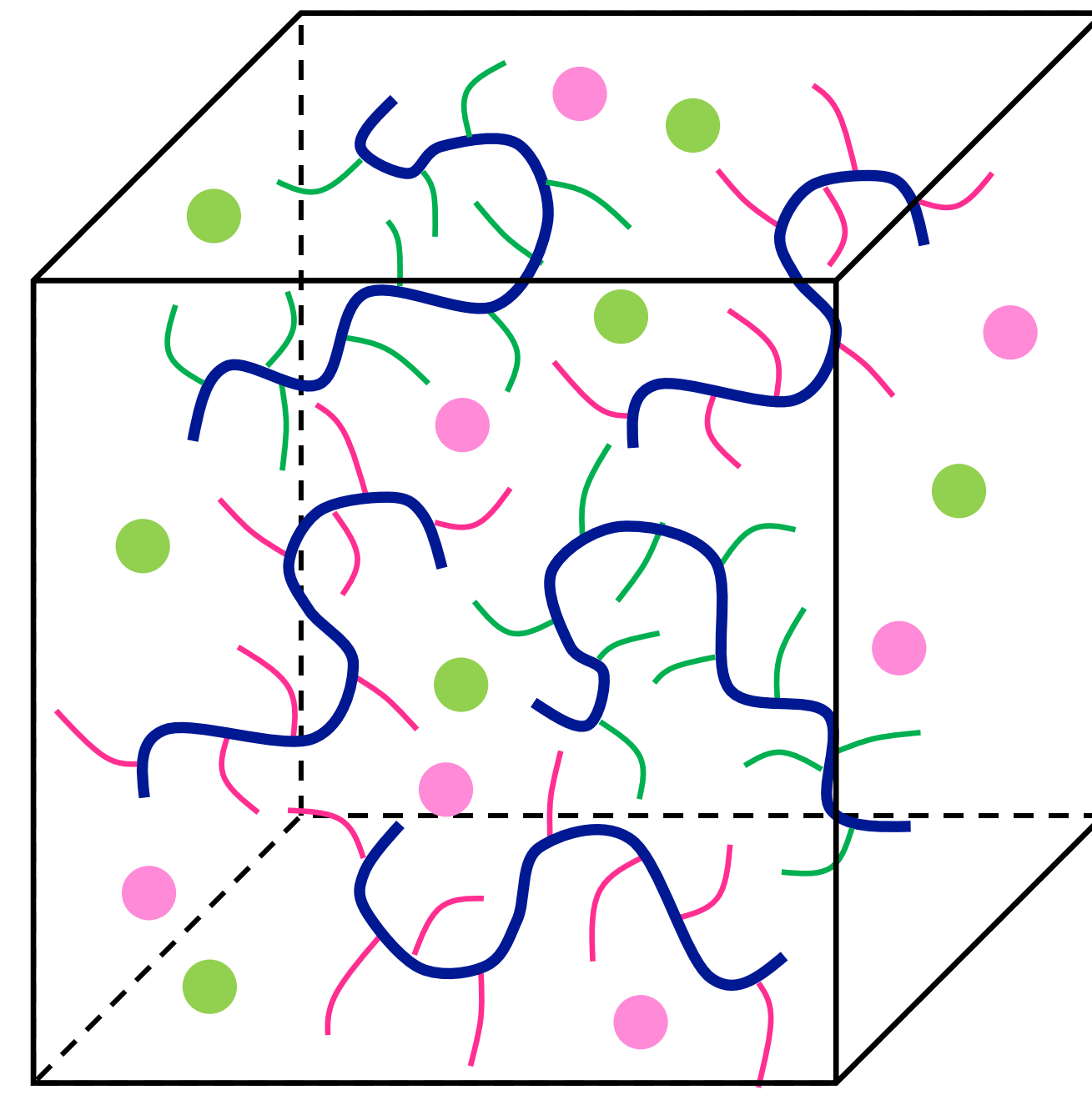
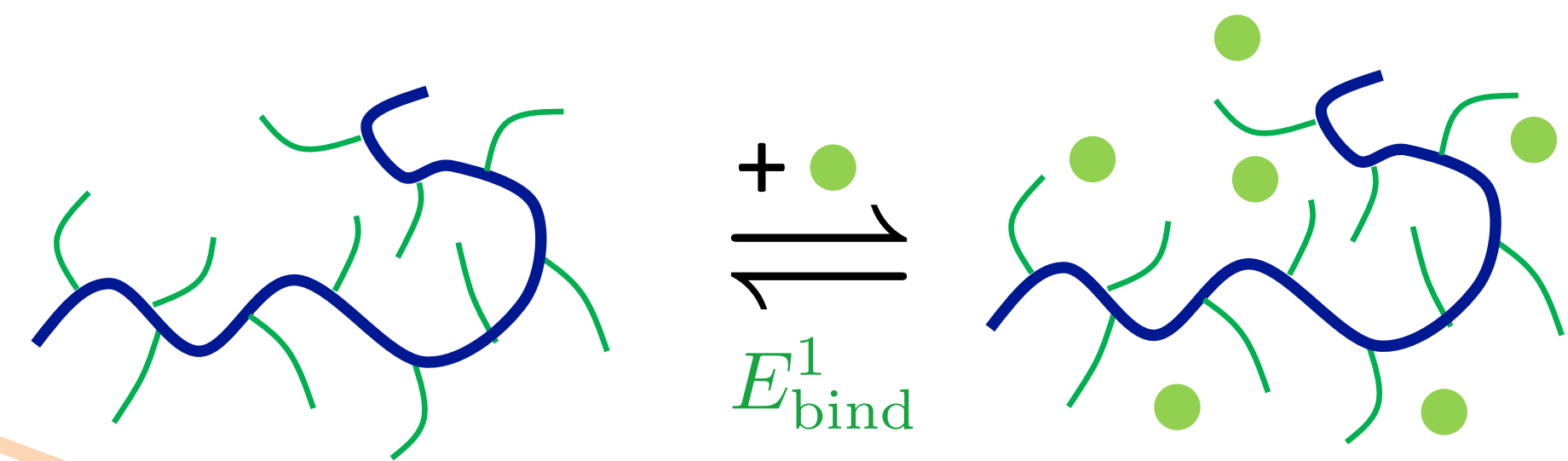


Polymer design for metal chelation¹

(in collaboration with Prof. Michael Schulz)

Polymers are promising candidates for metal ion extraction from complex solutions. Modelling can assist the design of such polymers by providing a fundamental understanding of the polymer-ion interaction at multiple time and length scales.



We develop parameters for the polarizable AMOEBA force field to accurately account for electrostatic effects. With classical molecular dynamics simulations, we can compute a binding affinity that includes both enthalpic and entropic contributions.



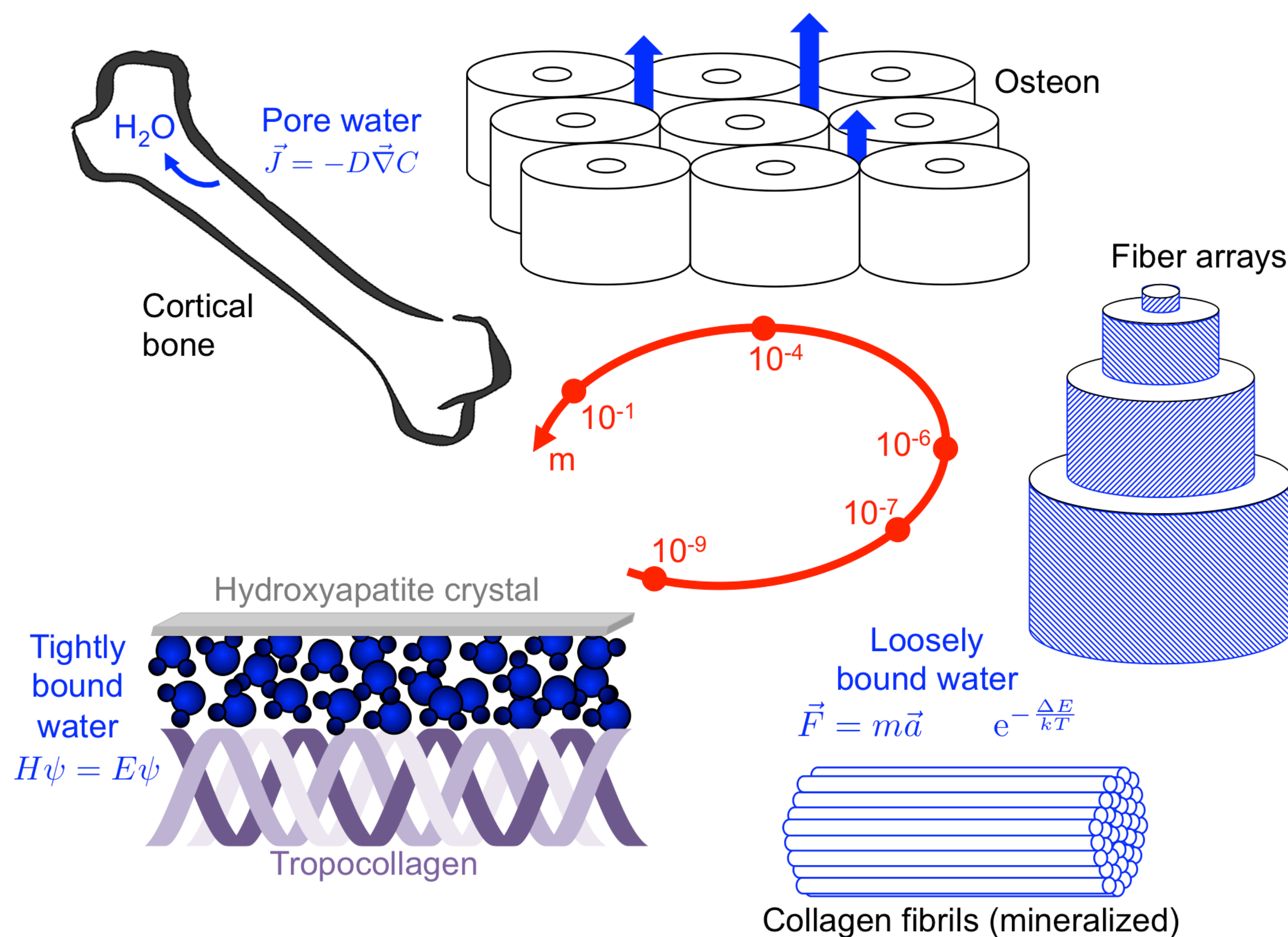
$$U^{\text{AMOEBA}} = U_{\text{bonded}} + U_{\text{vdW}} + U_{\text{ele}}^{\text{perm}} + U_{\text{ele}}^{\text{ind}}$$

Protein allostery²

Many biological processes, such as enzymatic catalysis and ion permeation through ion channels, rely on allosteric regulation. However, the molecular mechanisms of allosteric effects are poorly understood.

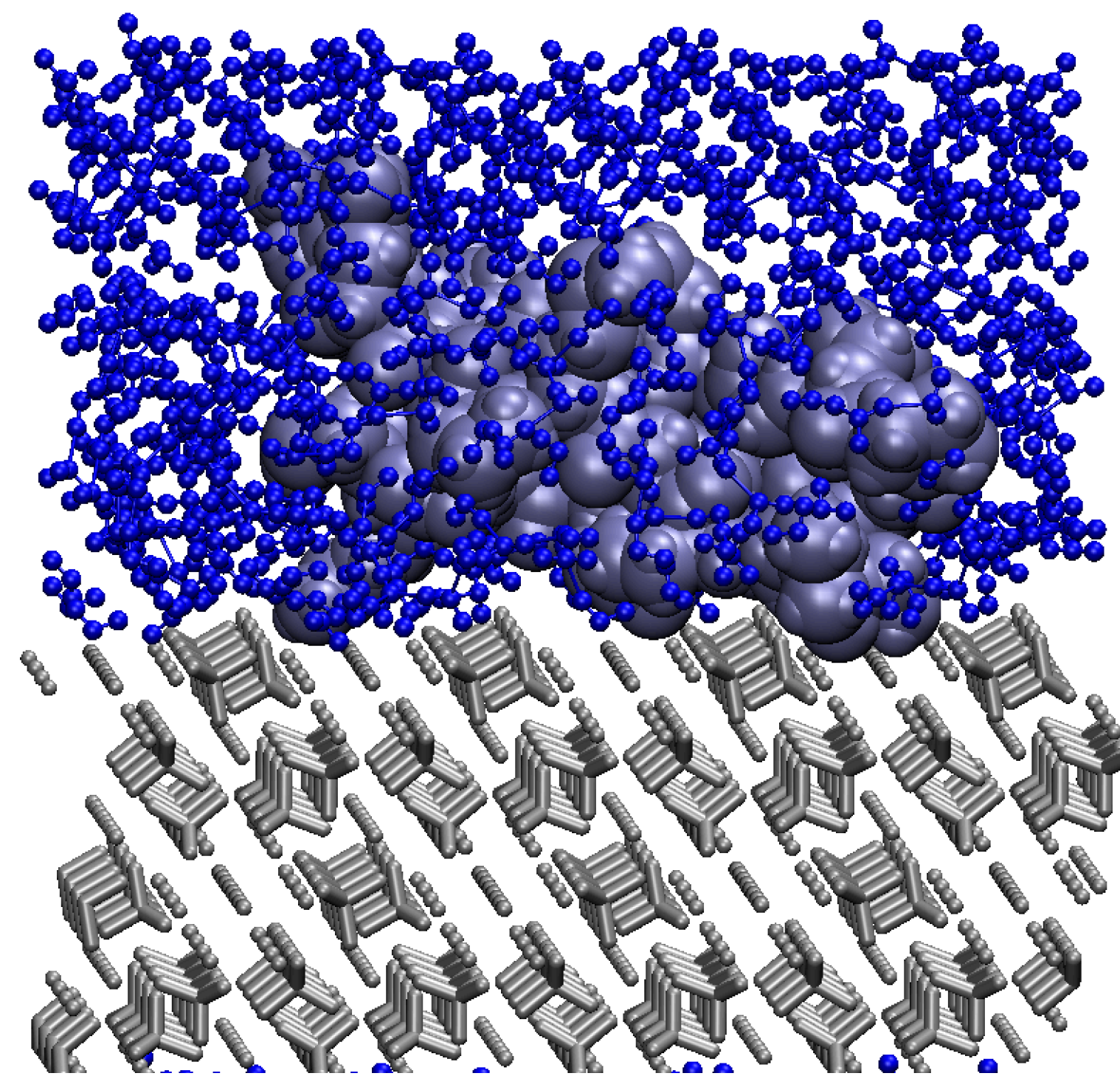
Water in cortical bone³

Bone's unique properties stem from the hierarchical organization of a mineral (hydroxyapatite) and an organic (collagen) phase across multiple length scales. A key player in the integration of the organic and inorganic components of bone is water.

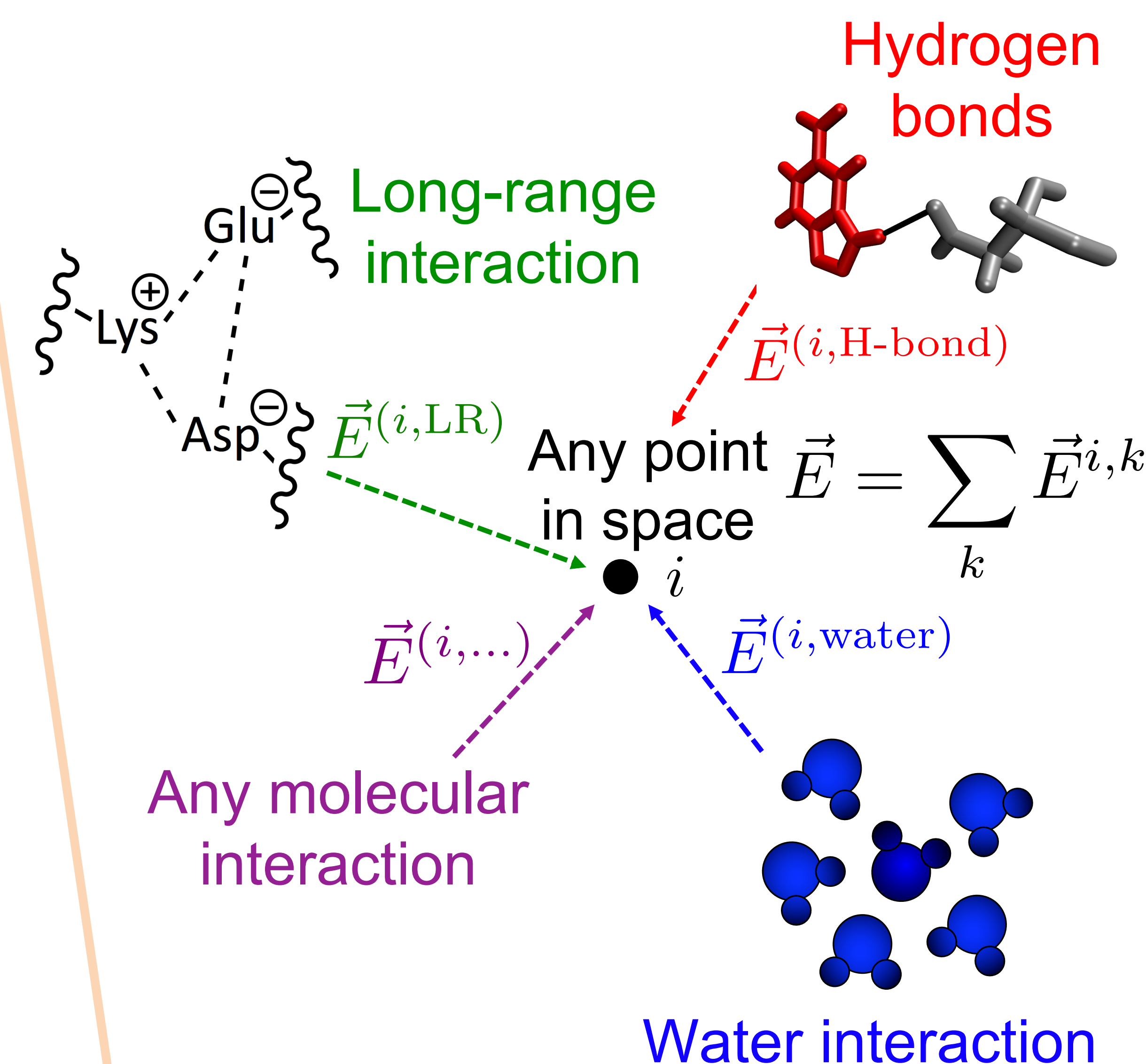
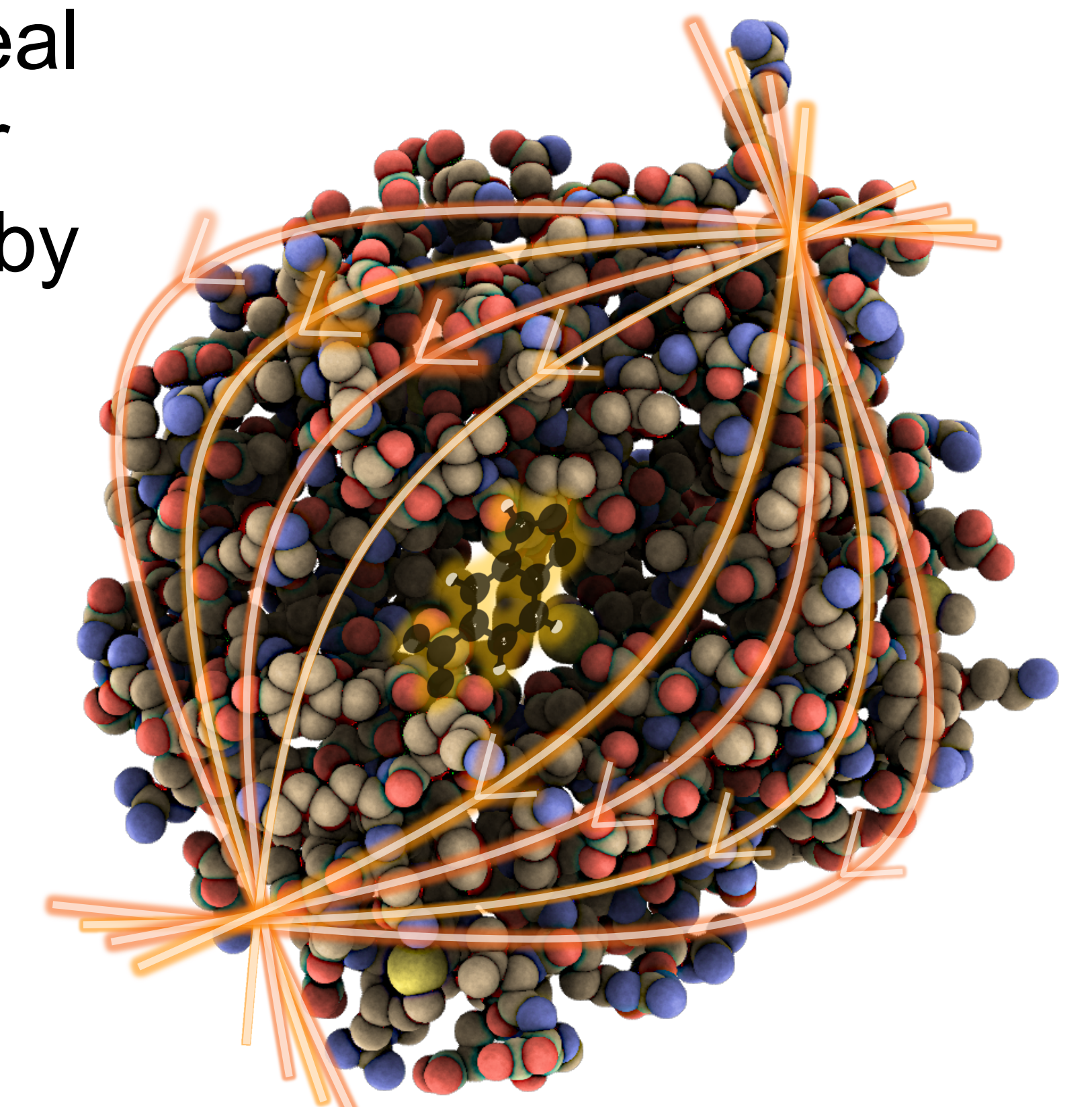


WELBORN GROUP

Molecular modeling of complex interfaces



Electric fields are an ideal probe for intermolecular interactions introduced by the environment for a target molecule (substrate, ions,...) modeled as a dipole.



Protein configurations of minimal energy are achieved by the best alignment of the substrate/ion dipole to the field they experience from their surroundings, which implicitly takes into account excluded volume, hydrogen bonding, and other noncovalent factors.

We contribute to the molecular understanding of the organization of organic and inorganic materials in bone. We use DFT MD to model this system and investigate the effects of confinement, collagen conformation and ionic concentration.

References

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- 2) V. Vaissier Welborn et al. Nat. Catal. 2018, 1, 649-655; V. Vaissier Welborn et al. J. Am. Chem. Soc. 2019, 141, 12487-12492
- 3) V. Vaissier Welborn et al. J. Phys. Chem. Lett. 2018, 1, 649-655; V. Vaissier Welborn et al. Nat. Commun. 2020, 11, 1-6.