

Supporting Information: Using Implicit-solvent Potentials to Extract Water Contributions to Enthalpy–Entropy Compensation in Biomolecular Association

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Short-range repulsion represented by modified WCA potential

Figure S1 shows the difference between $U_{\text{wca}(50,49)}$ and $U_{\text{wca}(12,6)}$ on representing the short-range repulsion. Clearly, $U_{\text{wca}(50,49)}$ is a better representation of the hard-core repulsion (an entropy effect), as its dominance in the short distances is affected less by the attraction term.

Different contributions to the interaction between two polymers

Figure S2 shows all the different contributions to the interaction between two disordered chains (left) and two folded chains (right), corresponding to the main text in Fig. 3A and Fig. 3C. Changes in U_{wca} and U_{bond} are very small compared to other components.

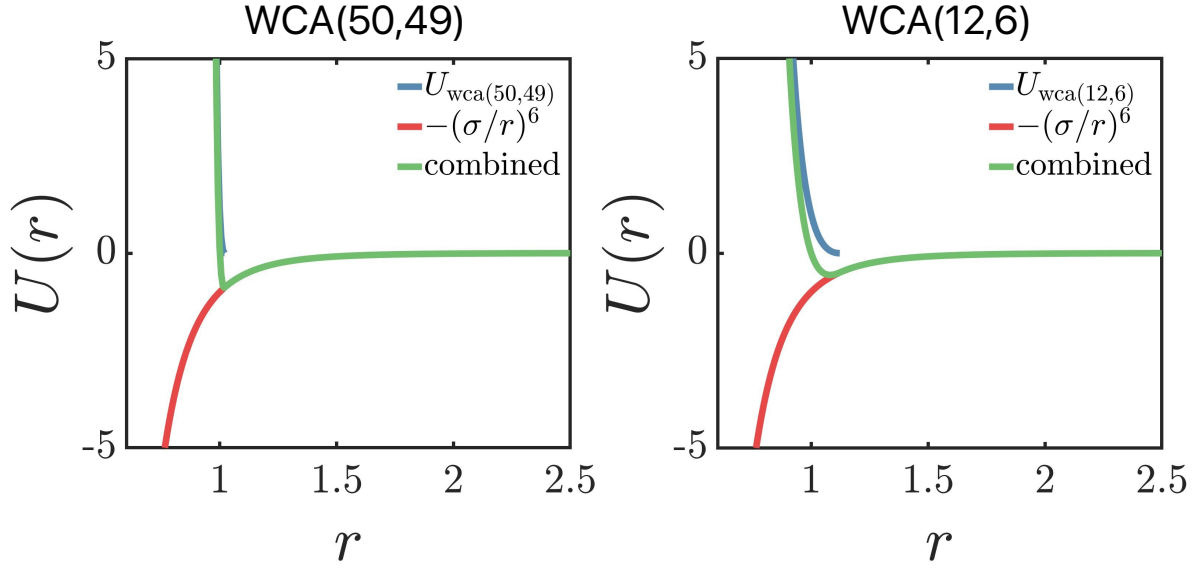


Figure S1: Difference between $U_{\text{wca}(50,49)}$ (blue curve, left) and $U_{\text{wca}(12,6)}$ (blue curve, right) in short-range repulsion.

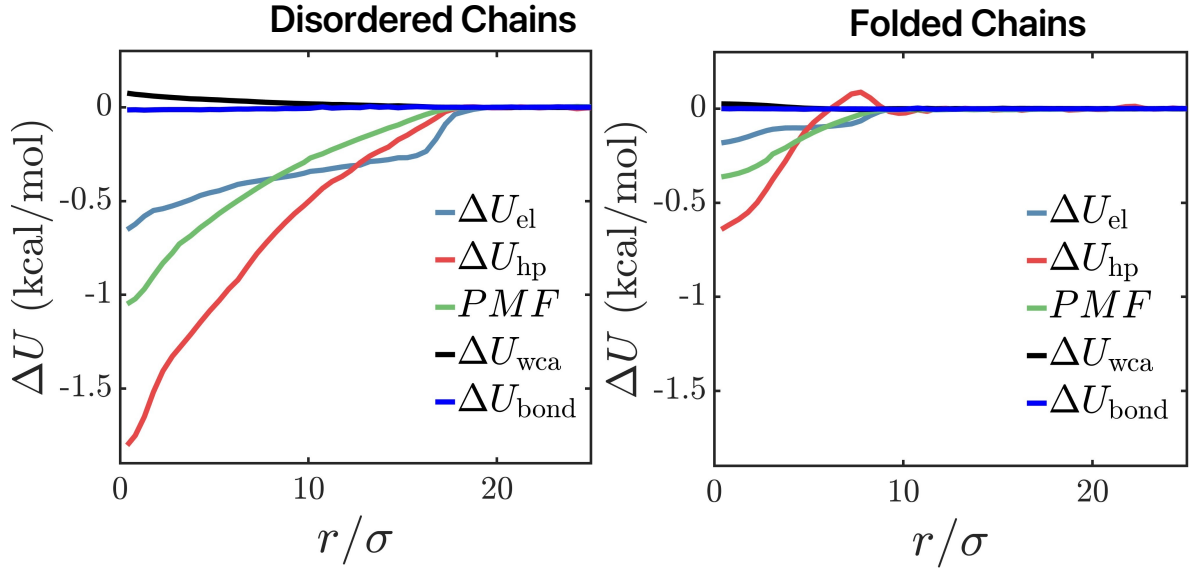


Figure S2: Different contributions to the interaction between two disordered chains (left), and between two folded chains (right).