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Membrane-mediated protein-protein interaction: A Monte Carlo study

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We investigate membrane-mediated interactions between transmembrane proteins using coarse-grained models. We compare the effective potential of mean force (PMF) between two proteins, which are always aligned parallel to the z-axis of the simulation box, with those PMFs obtained for proteins with fluctuating orientations. The PMFs are dominated by an oscillatory packingdriven contribution and a smooth attractive hydrophobic mismatch contribution, which vanishes if the hydrophobic length of the protein matches the thickness of the membrane. If protein orientations are allowed to fluctuate, the oscillations are greatly reduced compared to proteins with fixed orientation. Furthermore, the hydrophobic mismatch interaction has a smaller range. Finally, we compare the two-dimensional thickness profiles around two proteins with the predictions from the elastic theory of two coupled monolayers, and find them to be in very good agreement.

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