

A New Closure Theory for Describing Depletion of Molecules at Solid Interfaces

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Traditional density functional theories based on the classical closure relations are deficient in describing adsorption of fluids with severe depletion (deficit of molecules at the interface compared to the bulk phase). We develop a new bridge functional starting from more fundamental principles, i.e. basing on the third-order Ornstein-Zernike equation (OZ3) that improves over conventional liquid-theory closures (for example the hypernetted chain or the Percus-Yevick equations). Tests on the adsorption of Lennard-Jones fluid on planar hard walls show marked improvements and give quantitative agreement in the singlet density profiles.