73e Spatial Distribution and Aggregation of Water in a Reversed-Phase Liquid Chromatography System

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Various structural models for the stationary phase in a reversed-phase liquid chromatography (RPLC) system have been suggested from thermodynamic and spectroscopic measurements and theoretical considerations. To provide a molecular picture of a typical RPLC system, configurational-bias Monte Carlo simulations in the Gibbs ensemble are performed for a dimethyl octadecyl silanol bonded stationary phase on a model siliceous substrate in contact with mobile phases containing different methanol/water concentrations. It is shown that the alkyl chain conformation depends only weakly on the solvent composition. Residual surface silanol groups provide hydrogen bonding sites that lead to the formation of substrate bound water and methanol clusters, including bridging clusters that penetrate from the liquid interfacial region all the way to the silica surface.