Investigating Interfacial Structure and Retention in Reversed-Phase Liquid Chromatography

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Gibbs ensemble Monte Carlo simulations and the TraPPE force field are applied to model various reversed-phase liquid chromatography (RPLC) systems. These simulations provide unprecedented molecular-level insight on structure and retention. Results from simulations probing the effects of mobile phase composition (water/methanol and water/acetonitrile mixtures), the alkylsilane bonding density, the incorporation of polar embedded groups into the grafted chains, and the pore size on bonded-phase and interfacial structure and on solute retention will be reviewed. The simulations show that the RPLC stationary phase behaves significantly different than a bulk hydrocarbon phase and that both adsorption and partitioning play a key role in the retentive process.