1037-92-12 **P.W. Bates**, **G.W. Wei** and **Shan Zhao*** (szhao@bama.ua.edu), PO Box 870350, Department of Mathematics, University of Alabama, Tuscaloosa, AL 35487. *The Minimal molecular surface.*

In this talk, I will present a novel concept, the minimal molecular surface (MMS), as a new paradigm for the theoretical modeling of biomolecule-solvent interfaces. When a less polar macromolecule is immersed in a polar environment, the surface free energy minimization occurs naturally to stabilize the system, and leads to an MMS separating the macromolecule from the solvent. For a given set of atomic constraints (as obstacles), the MMS is defined as one whose mean curvature vanishes away from the obstacles. Based on the theory of differential geometry, an iterative procedure is proposed to compute the MMS via the mean curvature minimization of molecular hypersurface functions. Extensive numerical experiments, including those with internal and open cavities, are carried out to demonstrate the proposed concept and algorithms. Comparison is given to other space filling models, such as the molecular surface. Unlike the molecular surface, the proposed MMS is typically free of singularities. The application of the MMS to the electrostatic analysis is considered for a set of twenty six proteins. Some recent extensions of the molecular surface modeling via the constant mean curvature flow and a fourth order geometric flow will also be discussed. (Received November 05, 2007)