Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

The effect of macromolecular crowding on reaction rates: a computational and theoretical study[1] JUN SOO KIM, ARUN YETHIRAJ, Theoretical Chemistry Institute and Department of Chemistry, University of Wisconsin-Madison — The effect of macromolecular crowding on the rates of association reactions are investigated using theory and computer simulations. Reactants and crowding agents are both hard spheres, and when two reactants collide they form product with a reaction probability, p_{rxn}. A value of $p_{rxn} < 1$ crudely mimics the fact that proteins must be oriented properly in order for an association reaction to occur. The simulations show that the dependence of the reaction rate on the volume fraction of crowding agents varies with the reaction probability. For reaction probabilities close to unity where most of encounters between reactants lead to a reaction, the reaction rate always decreases as the volume fraction of crowding agents is increased due to the reduced diffusion coefficient of reactants. On the other hand, for very small reaction probabilities where in most of encounters the reaction does not occur, the reaction rate increases with the volume fraction of crowding agents, in this case, due to the increase probability of a re-collision. The Smoluchowski theory is in quantitative agreement with simulations for the reaction rate constant and allows the quantitative analysis of both effects separately.

[1]Supported by the National Science Foundation under Grant No. CHE-0717569.

Jun Soo Kim
Theoretical Chemistry Institute and Department of Chemistry,
University of Wisconsin-Madison

Date submitted: 18 Nov 2008 Electronic form version 1.4