

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Computer simulation of C60 permeation crossing dimyristoylphosphatidylethanolamine LIWEI LI, DMITRY BEDROV, GRANT SMITH, Department of Materials Science and Engineering, Department of Chemical Engineering, Utah — All-atom MD simulations have been carried out to investigate the permeation process of C60 crossing dimyristoylphosphatidylethanolamine(DMPC) lipid bilayer. The C60 has been constrained along the normal of bilayer from the surrounding water outside DMPC to the center of DMPC. The potential of mean forces(POMF) of C60 has been obtained by integrating the averaged forces acting on the C60. Local diffusion coefficient was calculated from the time autocorrelation function of instantaneous velocities. The overall resistance to C60 has been calculated in terms of POMF and the local diffusion coefficient. The C60 assembly behavior in the hydrophobic interior of DMPC was investigated by examining the POMF between two C60 molecules along lateral direction in the DMPC bilayer and in the bulk melt of alkyl chains.

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Date submitted: 30 Nov 2004

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