Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Molecular Dynamic Study to Determine the Ammonia Conduction Mechanisms in Human RhCG and Bacterial Homoloques UGUR AKGUN, Coe College — The transport of Ammonia is provided by Amt/MEP/Rh protein superfamily. The x-ray structures of AmtB from Escherichia coli, Rh50 from Nitrosomonas europaea, and human RhCG show only few differences on periplasmic vestibules. After more than microsecond simulation on three models, we determined the striking difference on conduction mechanism between bacterial AmtB and Human RhCG proteins. In AmtB the backbone carbonyl groups at the periplasmic vestibule direct charged ammonia to the conserved aromatic cage at the bottom of the vestibule. Furthermore, two partially stacked phenyl rings of F107 and F215, separating the periplasmic vestibule from the hydrophobic lumen, flip open and closed *simultaneously* with a frequency of approximately 108 flipping events per second. During the passage from the phenyl gates charged ammonia releases its proton and becomes gas. However, the absence of an aromatic cage on Rh proteins and a strongly conserved E166 residue in the vicinity hints different conduction mechanism. Our studies confirm the conserved E166 emerges as a strong charged ammonia recruitment site for Human RhCG. The conserved phenyl gate behaves different for Rh proteins and the synchronized motion is not observed. These findings suggest a different deprotonation mechanism than bacterial AmtB.

Ugur Akgun
Coe College

Date submitted: 15 Nov 2013 Electronic form version 1.4