Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Measurements of thermal and healing properties of nanoclay modified asphalt binders using molecular dynamics simulations DUSTIN BAKER, TAKUMI HAWA, The University of Oklahoma, ZAHID HOSSAIN, Arkansas State University, MRINAL SAHA, MUSHARRAF ZAMAN, The University of Oklahoma — A seven component molecular dynamics model has been developed to represent asphalt binder. The model has been developed to include the four major classes of molecules found in asphalt binders. The seven asphalt binder molecules were assembled with the Optimized Potentials for Liquid Simulations force field (OPLS) and the Large-scale atomic/molecular massively parallel simulator (LAMMPS) was used to carry out all simulations. Diffusion and density values were determined to validate individual molecules; all values were within acceptable range. Diffusion values were also determined for each molecule while present in the asphalt binder mixture. Density of the asphalt binder was determined to compare to experimental results. Values appear to follow the same trend as seen in experimental results and were closer to experimental results than other asphalt binder models. A glass transition temperature of 263.59K was determined using the density results at nineteen temperatures and was found to be in an acceptable range. A nano-clay model has also been developed using Clay force field and combined with the asphalt binder model. Also, we have investigated how the nano-clay impacts thermal and healing properties of the binder.

Takumi Hawa
The University of Oklahoma

Date submitted: 14 Nov 2013 Electronic form version 1.4