Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Morphology and chirality control self-assembly of sickle hemoglobin inside red blood cells[1] XUEJIN LI, HUAN LEI, Division of Applied Mathematics, Brown University, Providence, RI 02912, BRUCE CASWELL, School of Engineering, Brown University, Providence, RI 02912, GEORGE KARNIADAKIS, Division of Applied Mathematics, Brown University, Providence, RI 02912 — Sickle cells exhibit abnormal morphology and membrane mechanics in the deoxygenated state due to the polymerization of the interior sickle hemoglobin (HbS). In this study, the dynamics of self-assembly behavior of HbS in solution and corresponding induced cell morphologies have been investigated by dissipative particle dynamics approach. A coarse-grained HbS model, which contains hydrophilic and hydrophobic particles, is constructed to match the structural properties and physical description (including crowding effects) of HbS. The hydrophobic interactions are shown to be necessary with chirality being the main driver for the formation of HbS fibers. In the absence of chain chirality, only the self-assembled small aggregates are observed whereas self-assembled elongated step-like bundle microstructures appear when we consider the chain chirality. Several typical cell morphologies (sickle, granular, elongated shapes), induced by the growth of HbS fibers, are revealed and their deviations from the biconcave shape are quantified by the asphericity and elliptical shape factors.

[1]This work was supported by the National Institutes of Health (NIH) Grant R01HL094270 and the National Science Foundation (NSF) Grant CBET-0852948.

Xuejin Li
Brown University

Date submitted: 11 Nov 2011 Electronic form version 1.4