

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Conformational response of a clay binding protein (EGF) by a coarse-grained Monte Carlo simulation¹ BARRY FARMER, LAWRENCE DRUMMY, RAJESH NAIK, Air Force Research Laboratory, MADHAVI KADAKIA, Wright State University, RAS PANDEY, University of Southern Mississippi — Biofunctionalization of montmorillonite (MMT) clay platelets with epidermal growth factor (EGF) appears to play a critical role in tissue regeneration (cell growth and migration) [1]. How the protein (EGF) binds to clay platelet and conforms is very important in its ability to activate the epidermal growth factor receptor. It is however difficult to monitor such structural response systematically in a current laboratory setting. We investigate the structural response of the protein EGF as it binds to the clay platelet with a coarse-grained model already used to investigate binding of short peptides. Both the EGF protein and the clay platelets are described by nodes tethered together by fluctuating covalent bonds. Each residue interacts with a phenomenological interaction (based on its hydrophathy index). Protein and platelet perform their stochastic motion with the Metropolis algorithm. A number of local (e.g. mobility and structural profiles) and global physical quantities such as gyration radius are examined as a function of temperature. We are able to identify the immobilized segments of protein and the variation of its size as a function of temperature. [1] C.A. Vaiana et al Biomacromolecules xxx (2011)

¹This work is supported by the Air Force Research Laboratory.

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Date submitted: 08 Nov 2011

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