Abstract Submitted
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Modeling Shear Induced Von Willebrand Factor Binding to Collagen[1] CHUQIAO DONG, WEI WEI, MICHAEL MORABITO, EDMUND WEBB, ALPARSLAN OZTEKIN, XIAOHUI ZHANG, XUANHONG CHENG, Lehigh Univ — Von Willebrand factor (vWF) is a blood glycoprotein that binds with platelets and collagen on injured vessel surfaces to form clots. VWF bioactivity is shear flow induced: at low shear, binding between VWF and other biological entities is suppressed; for high shear rate conditions as are found near arterial injury sites VWF elongates, activating its binding with platelets and collagen. Based on parameters derived from single molecule force spectroscopy experiments, we developed a coarse-grain molecular model to simulate bond formation probability as a function of shear rate. By introducing a binding criterion that depends on the conformation of a sub-monomer molecular feature of our model, the model predicts shear-induced binding, even for conditions where binding is highly energetically favorable. We further investigate the influence of various model parameters on the ability to predict shear-induced binding (vWF length, collagen site density and distribution, binding energy landscape, and slip/catch bond length) and demonstrate parameter ranges where the model provides good agreement with existing experimental data. Our results may be important for understanding vWF activity and also for achieving targeted drug therapy via biomimetic synthetic molecules.

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