Supporting Information for

Bilirubin oxidase adsorption onto charged self-assembled monolayers: Insights from multiscale simulations

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The number of pages: 4

The number of figures: 4

The number of tables: 1

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Table S1. The key adsorption residues of MvBOx adsorbed on charged surfaces.

system	The main adsorption residues
MvBOx on HOOC-SAM（7%）	Thr348, Gln351, Arg353, Arg356, Thr357, Gly358, Gly365, Asn394, Gly415, Asn416, Arg437
MvBOx on HOOC-SAM（25%）	Arg353, Arg356, Thr357, Gly358, Asn364, Gly365, Val366Asp370, Gln372, Asn373, Asn394, Arg437
MvBOx on NH_2-SAM（7%）	Val13, Pro14, Gln22, Thr47, Gln49, Pro52, Asp53, Gly55, Ser56, Phe213, Asn215, Asp322, Asp323, Thr325, Gln505, Ala506, Gln507, Ser508, Val513, Gln514
MvBOx on NH_2-SAM（25%）	Pro14, Gln22, Pro52, Asp53, Phe172, Asp322, Asp323, Thr324, Thr325, Gln505, Ala506, Gln507

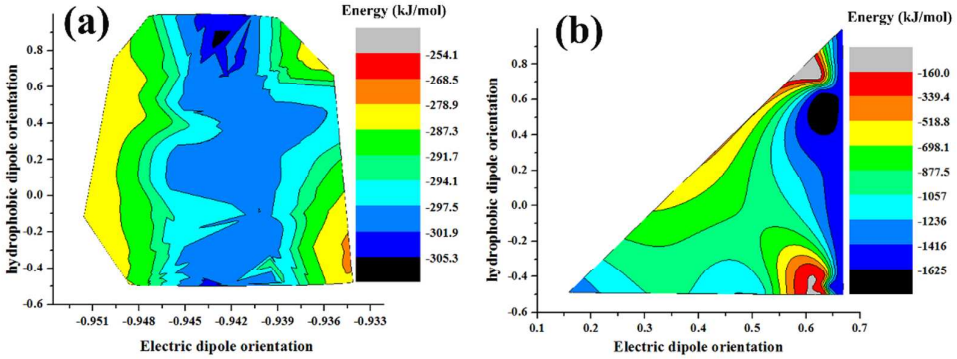

Figure S1 Interaction energies versus electric dipole and hydrophobic dipole of MvBOx in PTMC sampling. (a) MvBOx on the positively charged surface; (b) MvBOx on the negatively charged surface.

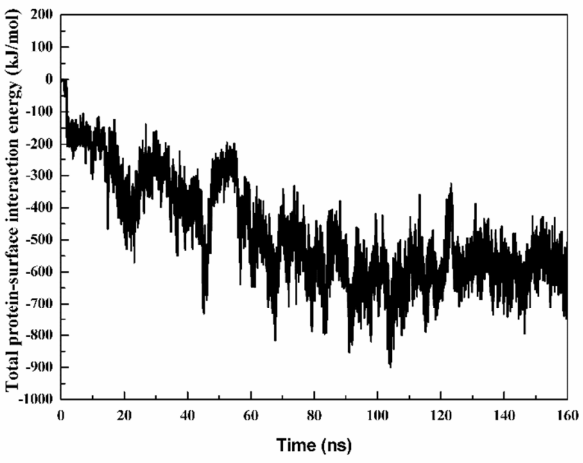

Figure S2. The time evolution of total protein-surface interaction energy during the MD simulation

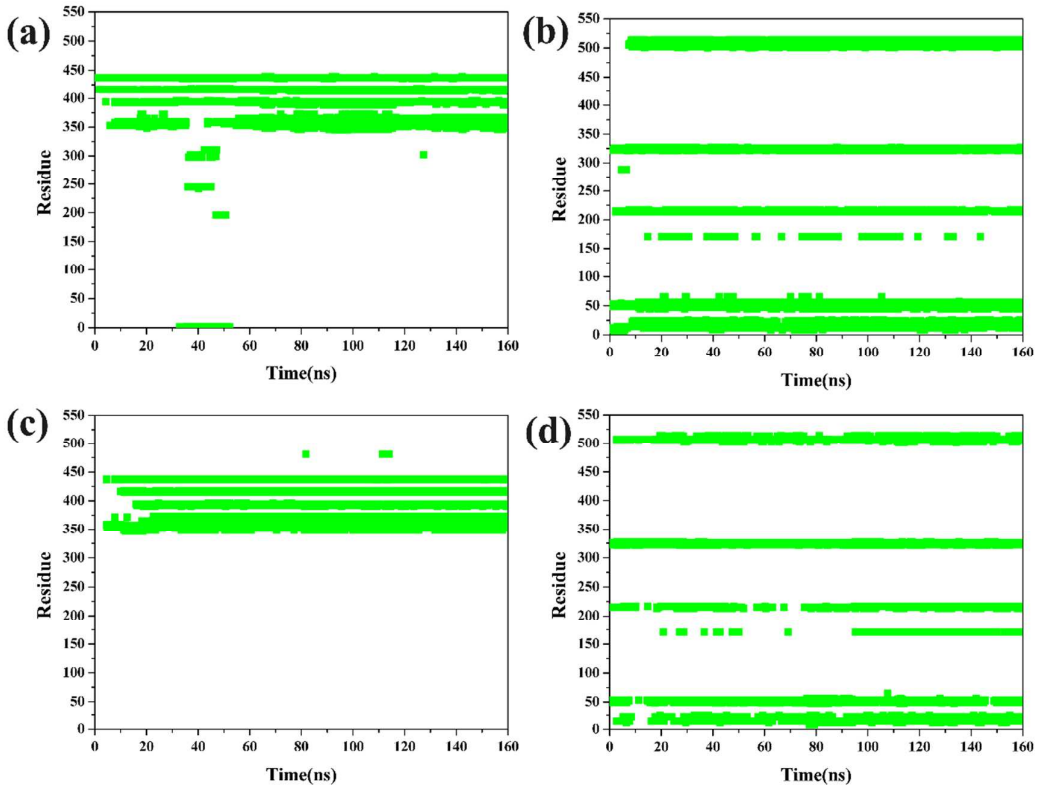

Figure S3. Contact maps between MvBOx and charged SAMs during simulations: (a) 7% dissociated COOH-SAM; (b) 7% dissociated NH_2-SAM; (c) 25% dissociated COOH-SAM; (d) 25%

dissociated NH_2-SAM.

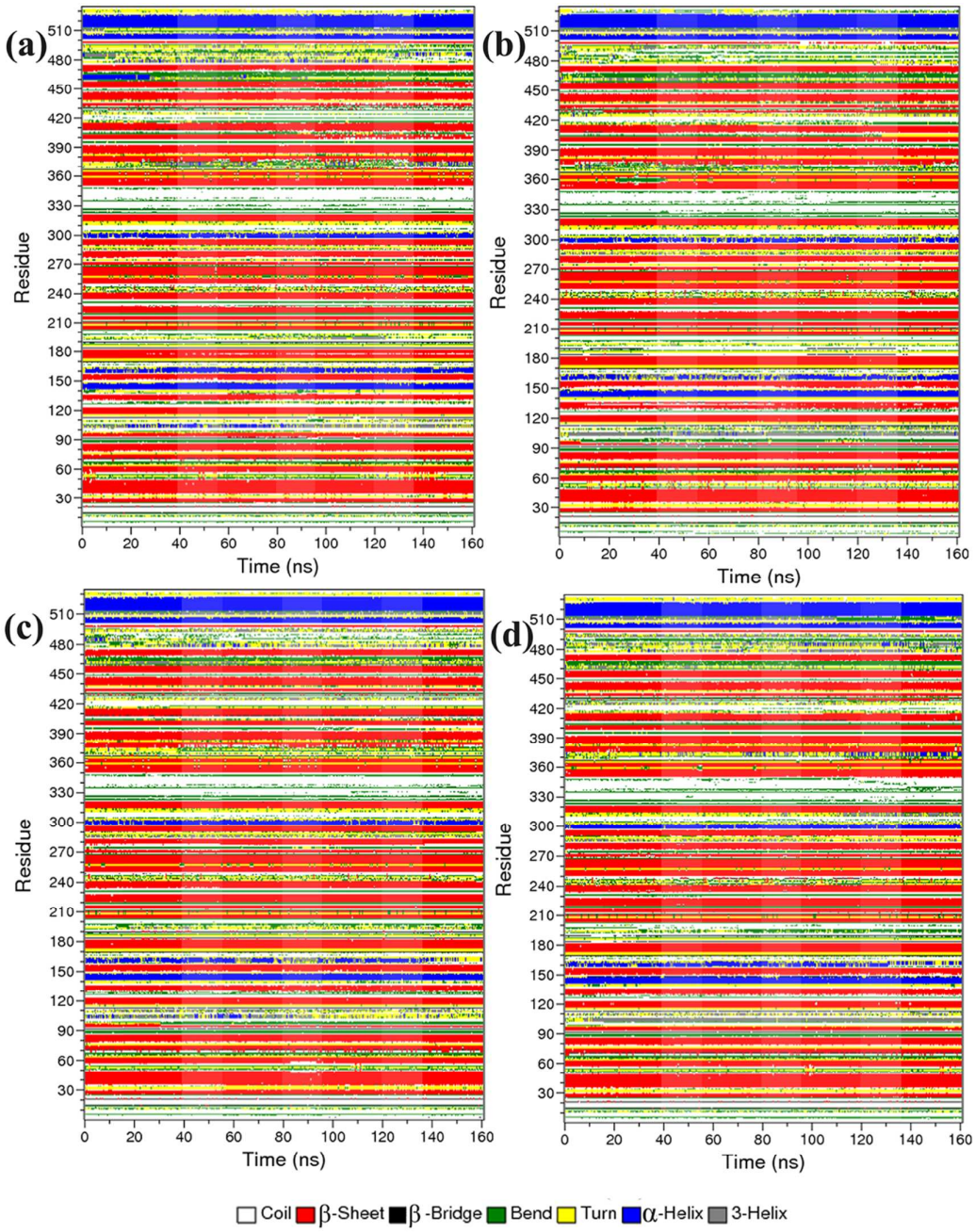

Figure S4. Time evolution of the secondary structures of MvBOx adsorbed on different charged surfaces: (a) on 7% dissociated COOH-SAM; (b) on 7% dissociated NH_2-SAM; (c) on 25% dissociated COOH-SAM; (d) on 25% dissociated NH_2-SAM.