

Supporting Information

Effect of substrate charge density on the adsorption of intrinsically disordered protein amyloid β 40: A molecular dynamics study[†]

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S1. Secondary structural analysis

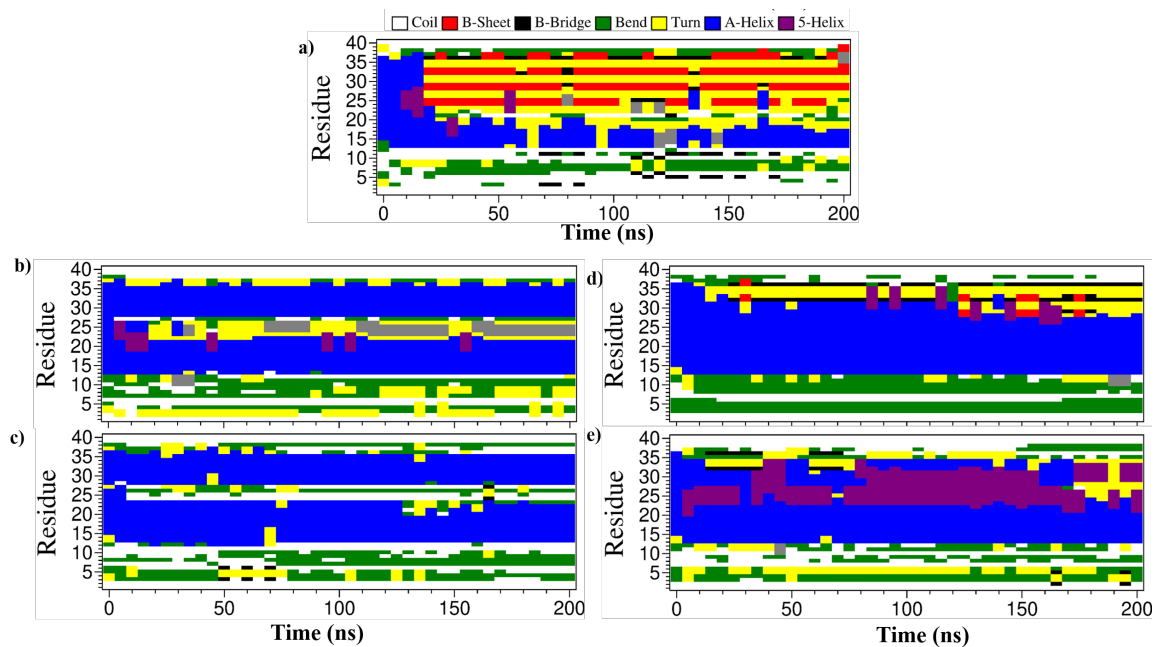


Figure S1: Time evolution of secondary structure of A β 40 for different system by DSSP analysis. (a) CP (b) 0.0, (c) -0.033, (d) -0.100, (e) -0.167 e/nm^2

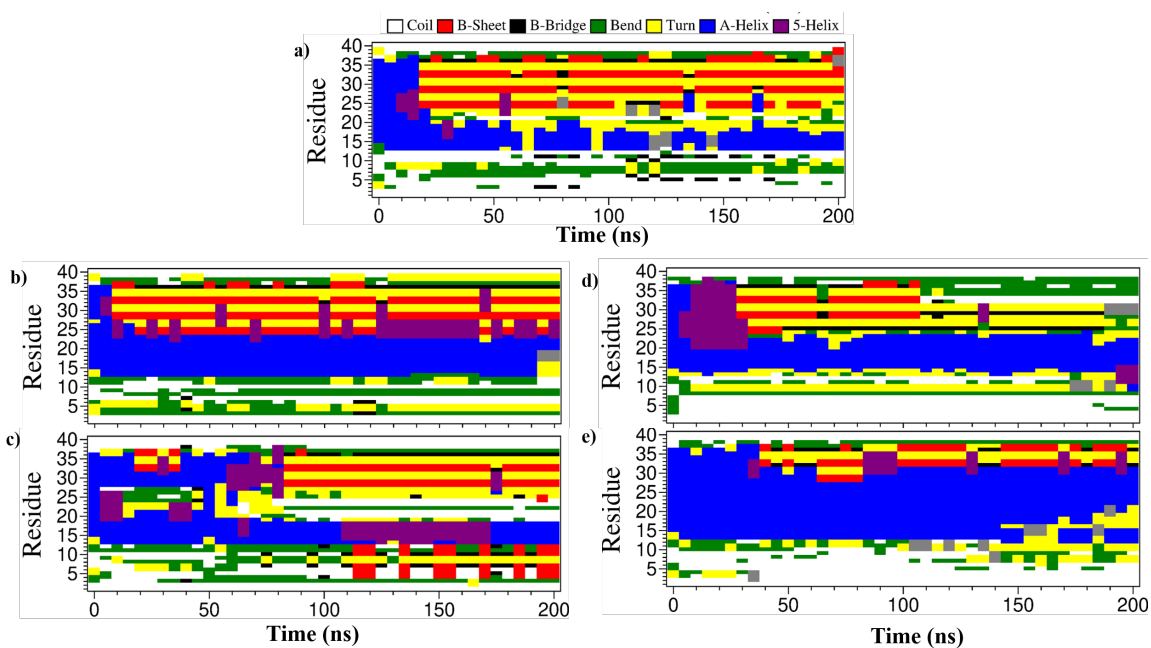


Figure S2: Time evolution of secondary structure of A β 40 for different system by DSSP analysis. (a) CP (b) -0.234 (c) -0.267 (d) -0.300 (e) -0.334 (e/nm²)

S2. Comparison of H-REMD and normal MD

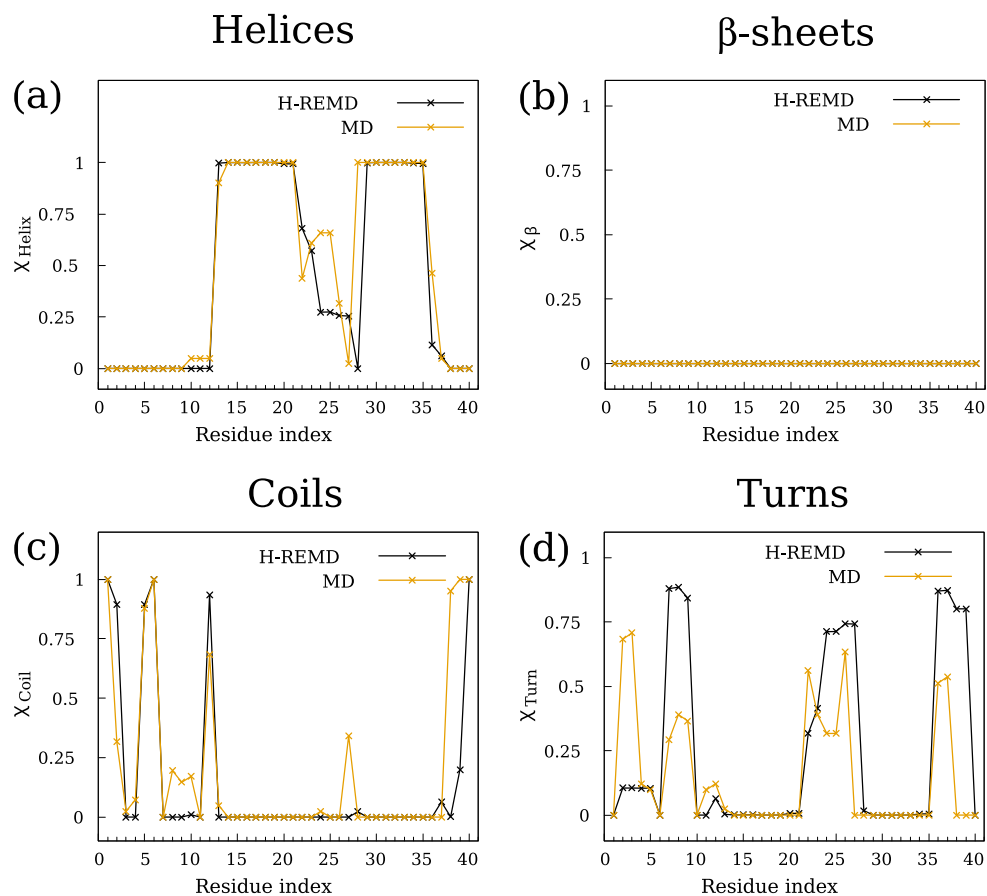


Figure S3: Fraction of (a) helices, (b) β -sheets, (c) coils, and (d) turns as a function of residue index for A β 40 on neutral Au slab.

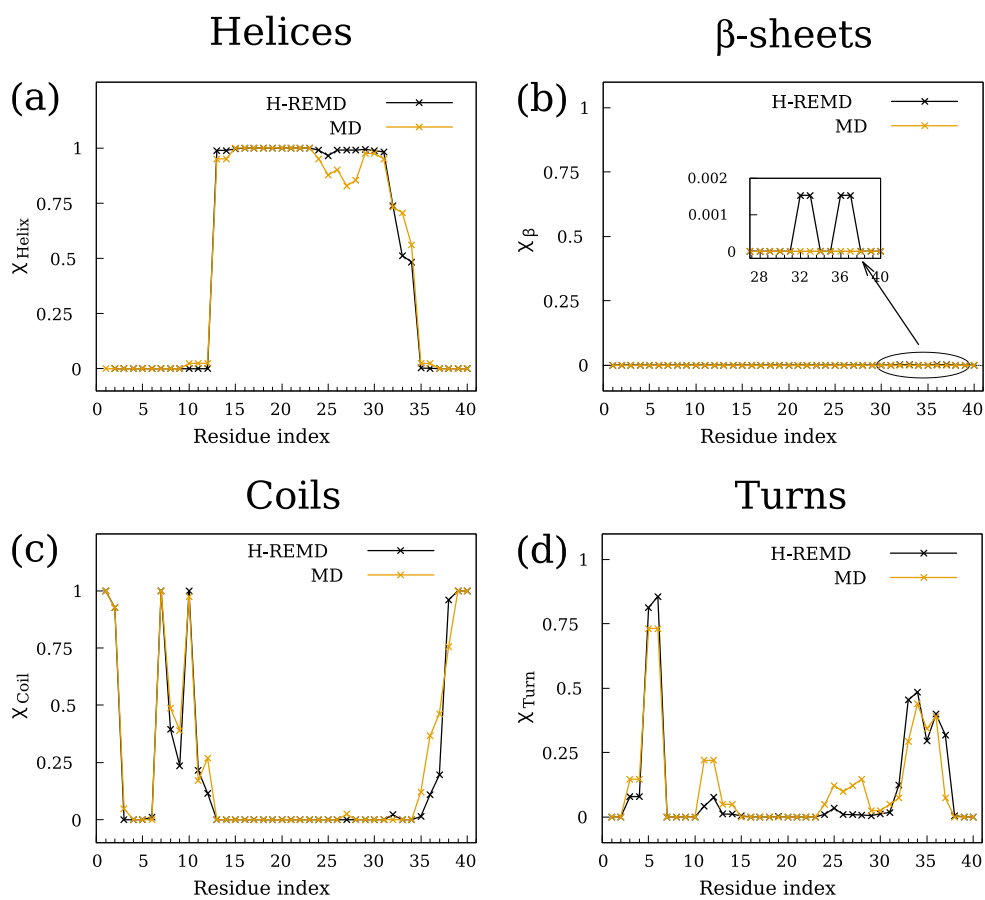


Figure S4: Fraction of (a) helices, (b) β -sheets, (c) coils, and (d) turns as a function of residue index for A β 40 on negatively charged (-0.167 e/nm^2) Au slab.

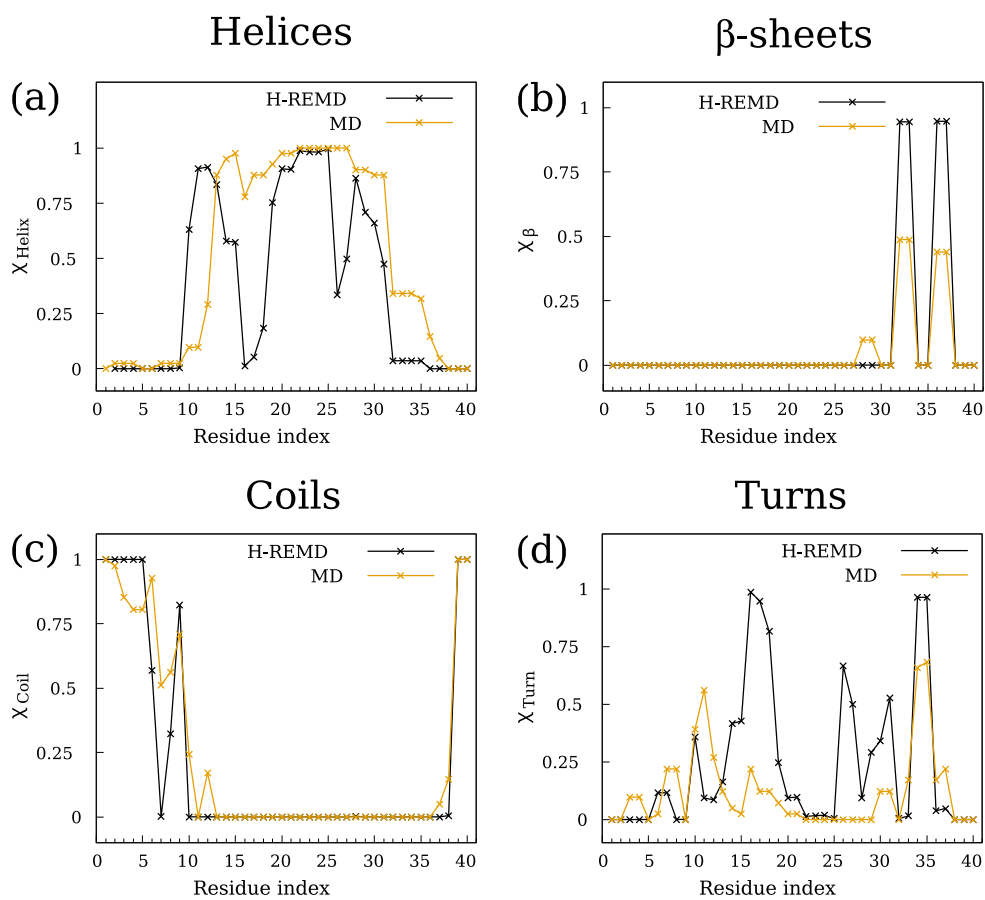


Figure S5: Fraction of (a) helices, (b) β -sheets, (c) coils, and (d) turns as a function of residue index for A β 40 on negatively charged (-0.334 e/nm^2) Au slab.

S3. Counterion condensation

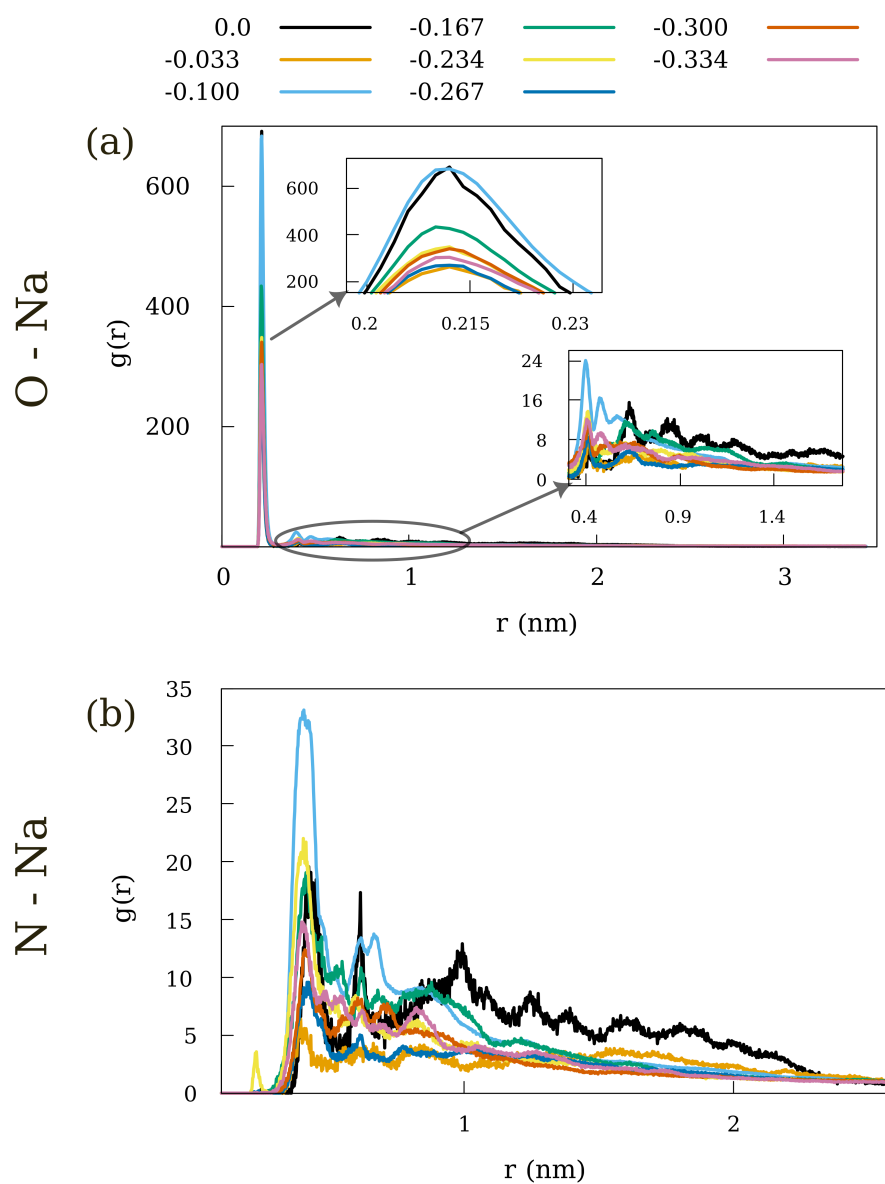


Figure S6: Radial distribution function between (a) $O^{\delta-}$ and Na^+ , and (b) $N^{\delta-}$ and Na^+ .

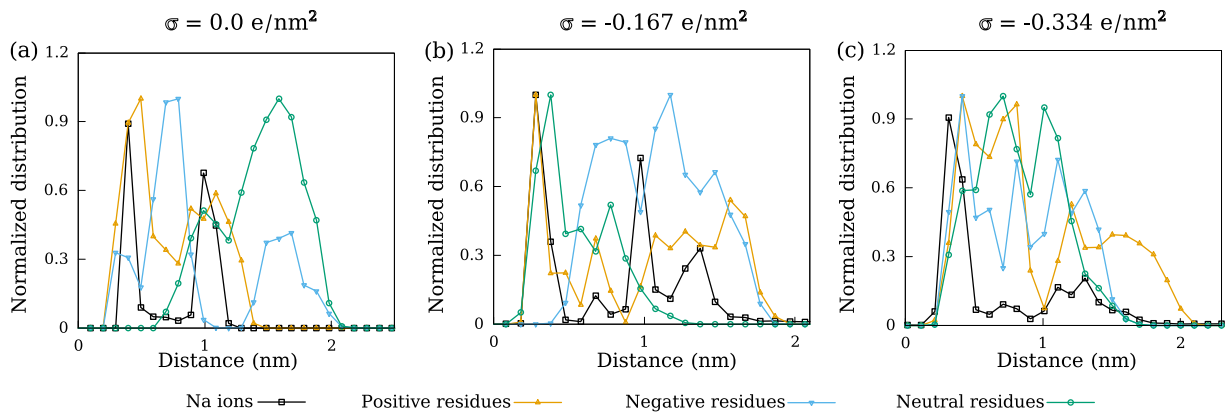


Figure S7: Planar normalized distribution of counterions (Na), positively charged residues, negatively charged residues, and neutral residues are shown for (a) $\sigma = 0.0 \text{ e/nm}^2$, (b) -0.167 e/nm^2 , (c) -0.334 e/nm^2 . Since the number density is different for each atoms/residues, we have normalized them individually.