Supplementary Information (SI) for Nanoscale.

Predicting Biomolecule Adsorption on Nanomaterials: A Hybrid Framework of Molecular Simulations and Machine Learning

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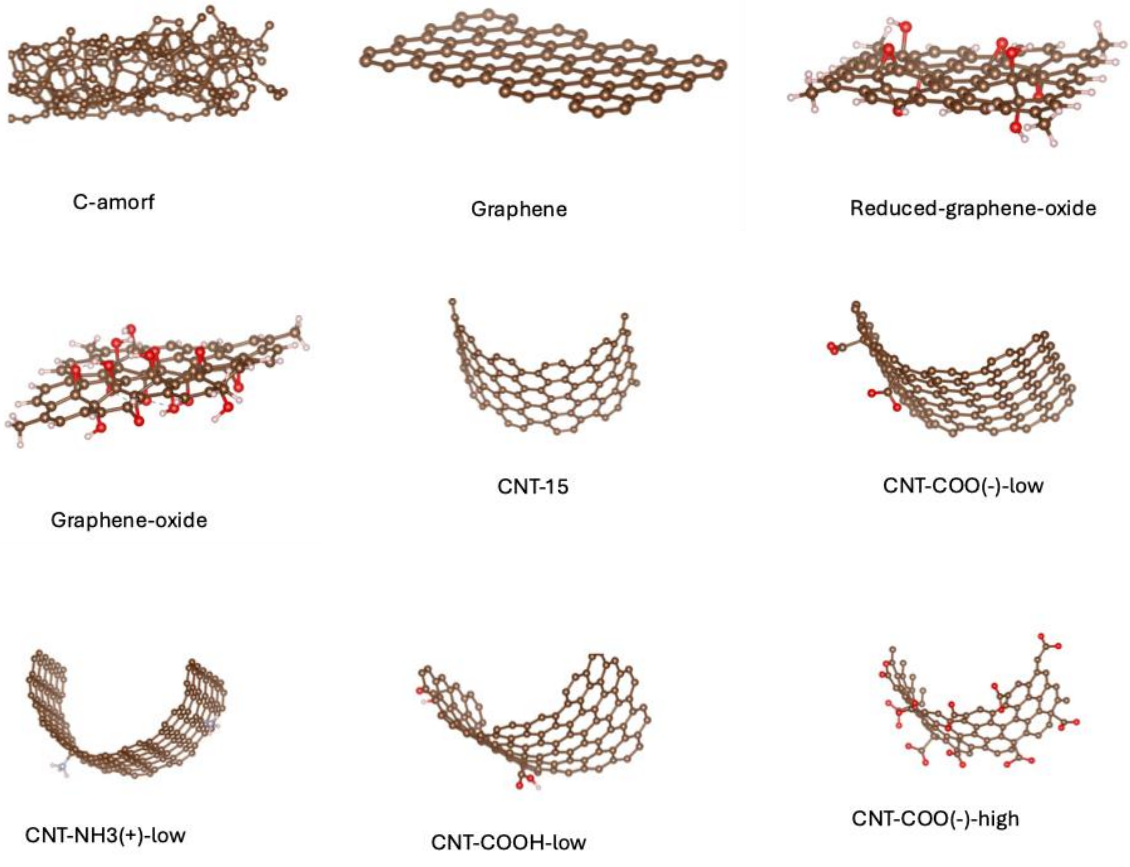
Supplementary materials

1. Structural representation of nanomaterials (NMs) used in meta-modeling:

A. Carbon-based NMs

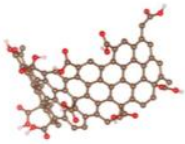


CNT-NH2-low

CNT-NH2-high

CNT-OH-low

CNT-OH-high

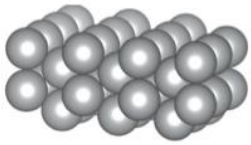


CNT-COOH-high

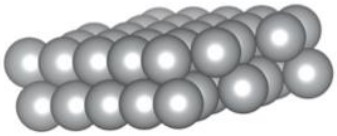
CNT-NH3(+)-high

B. Metals NMs

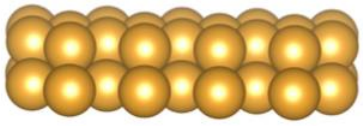
Ag100



Ag110

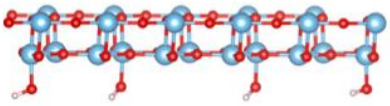


Ag111

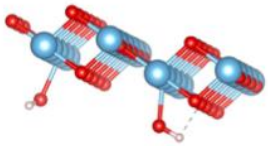


Au100

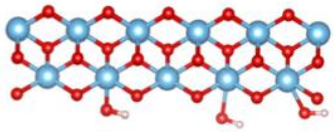
C. Metal oxides NMs



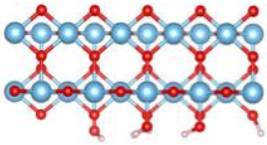
Anatase-OH-100



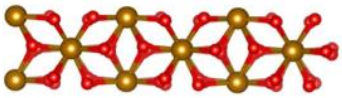
Anatase-OH-101



Rutile-OH-100

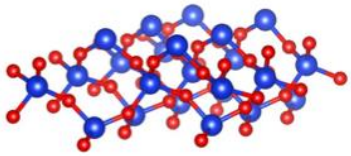


Rutile-OH-110

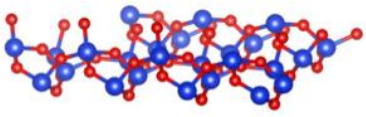


Fe2O3

D. Metalloid oxide NMs

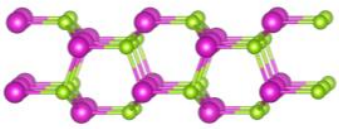


SiO2-amorph



SiO2-quartz

E. Cedmium selenide NMs



CdSe-2m10