

Electronic Descriptors and Periodic Trends in Graphene/LDH-Based Nanocarriers for Breast Cancer Drug Delivery

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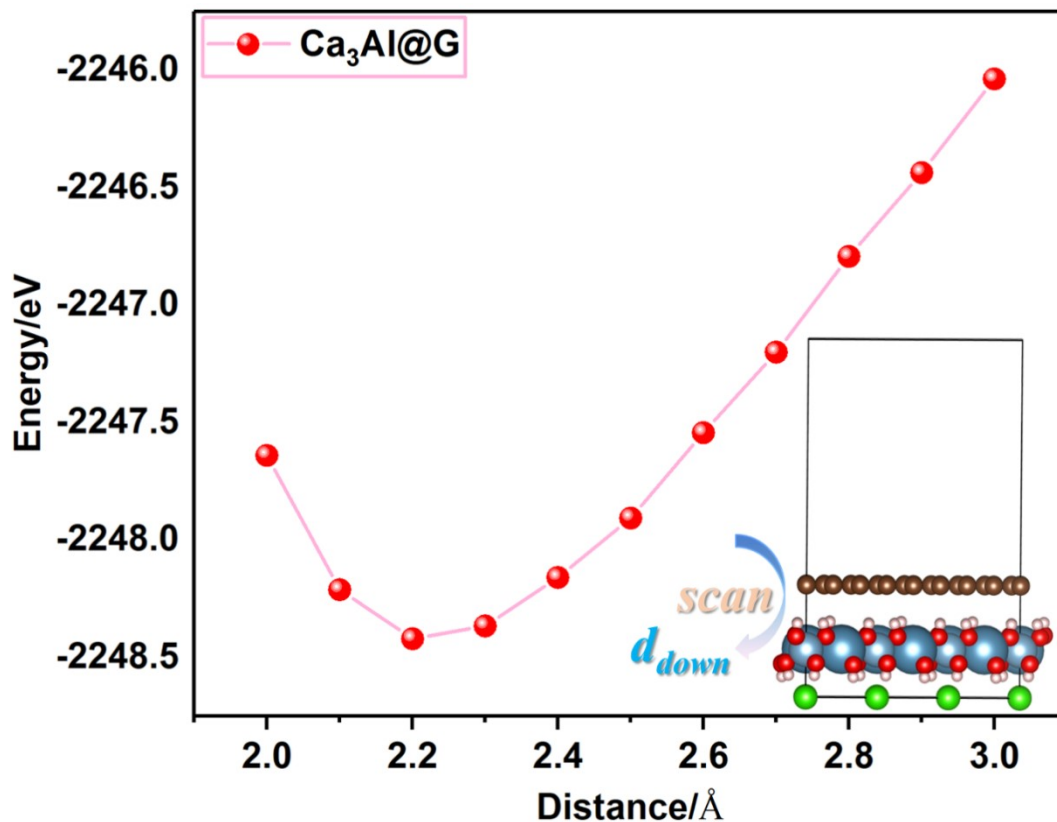


Figure S1. Potential energy surface scans for heterobilayer graphene/ Ca_3Al -LDHs systems are performed based on the distance between graphene and Ca_3Al -LDHs.

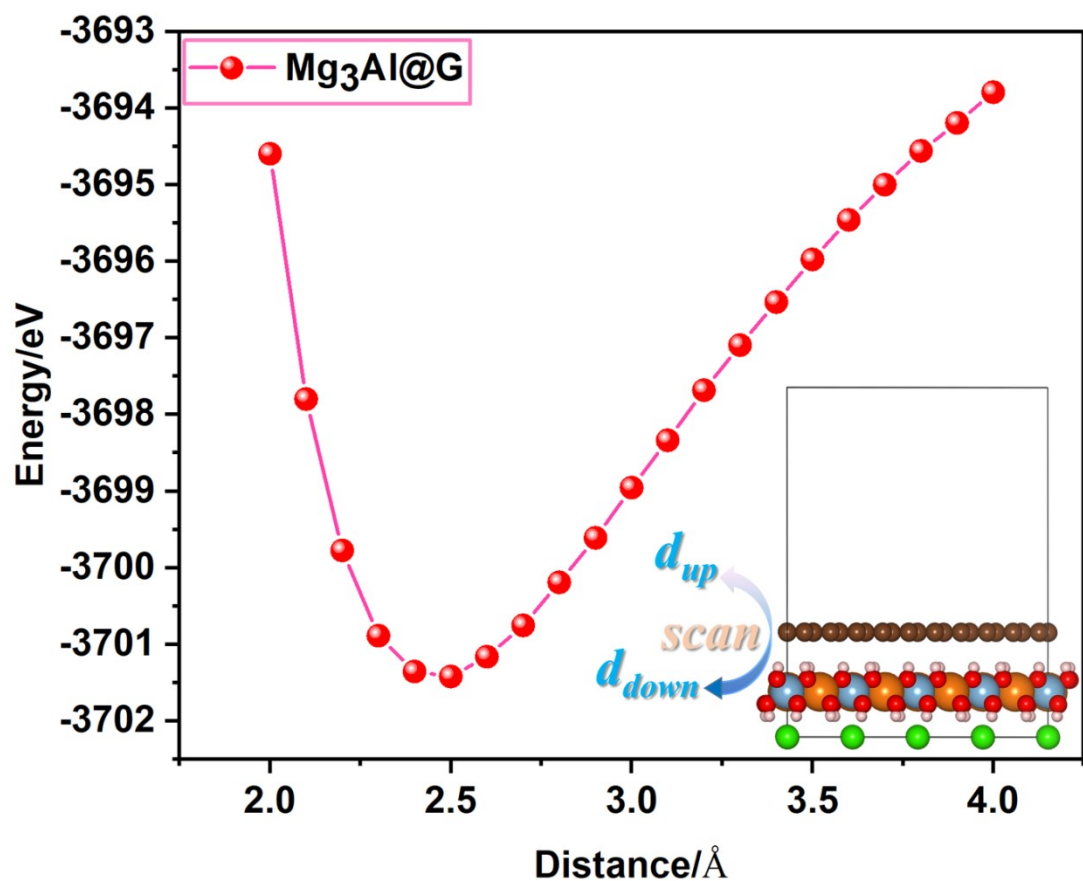


Figure S2. Potential energy surface scans for heterobilayer graphene/ Mg_3Al -LDHs systems are performed

based on the distance between graphene and Mg₃Al-LDHs.

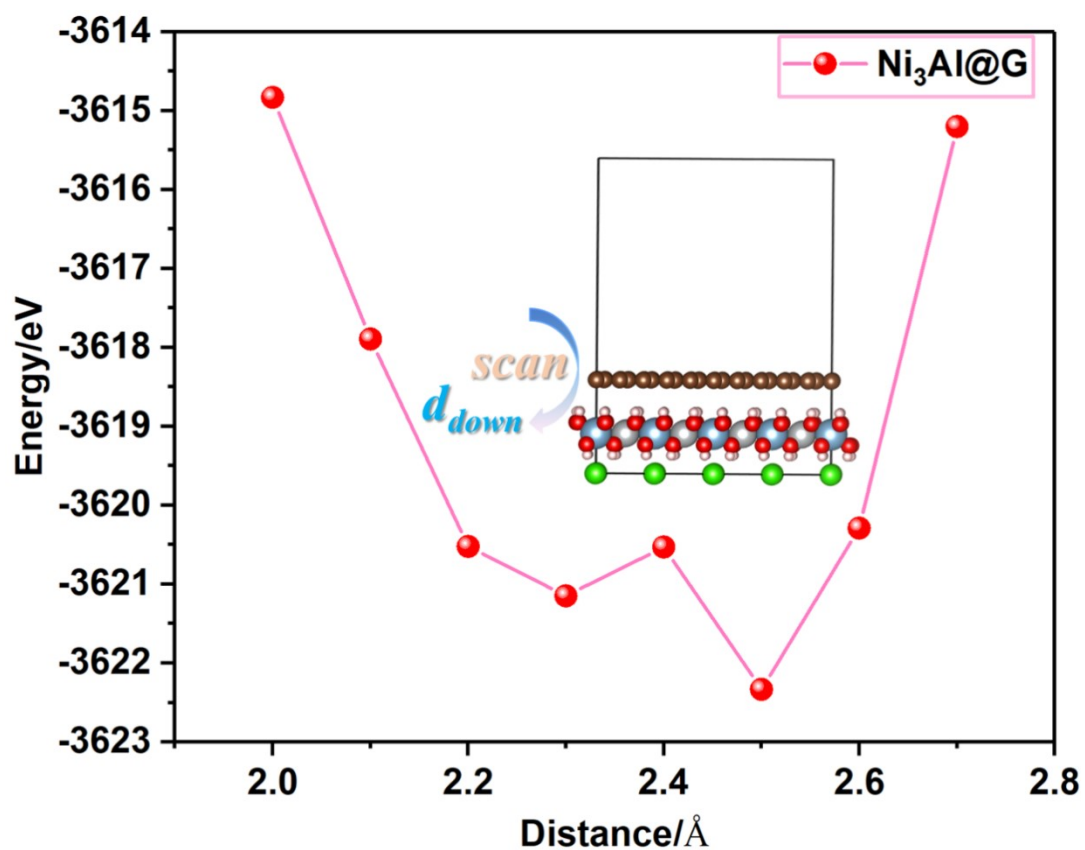


Figure S3. Potential energy surface scans for heterobilayer graphene/Ni₃Al-LDHs systems are performed based on the distance between graphene and Ni₃Al-LDHs.

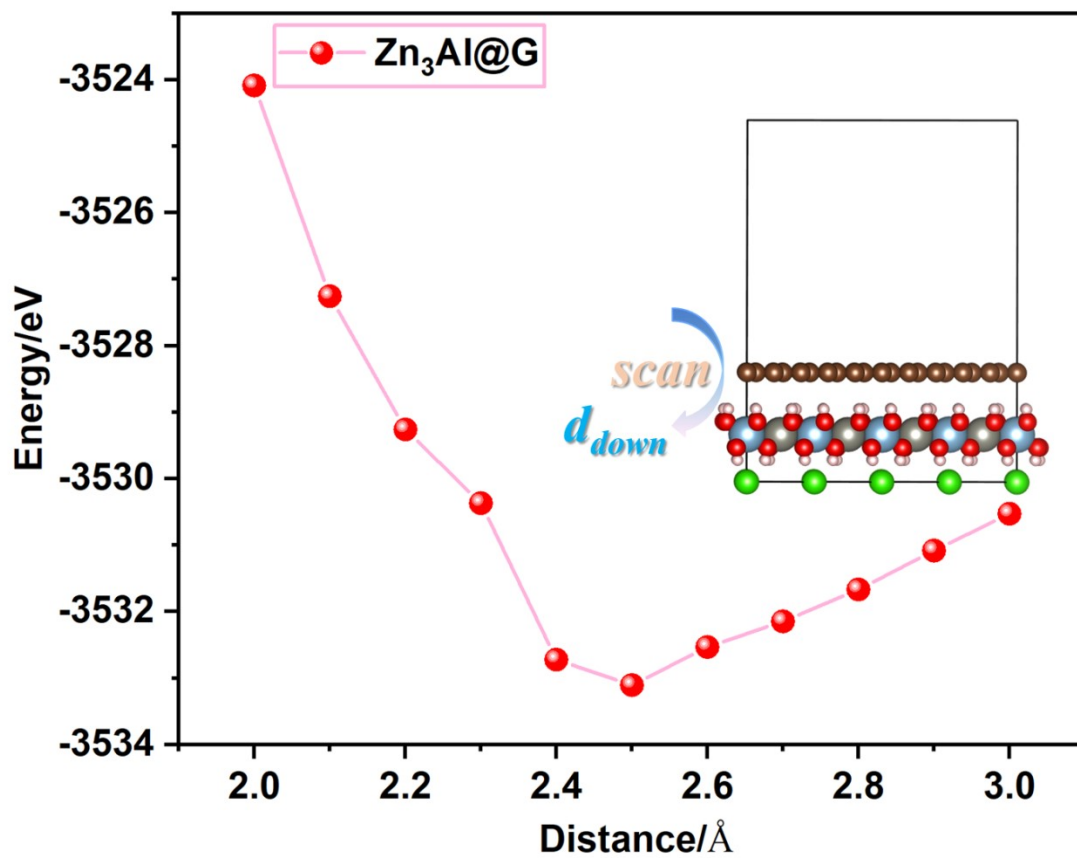


Figure S4. Potential energy surface scans for heterobilayer graphene/Zn₃Al-LDHs systems are performed based on the distance between graphene and Zn₃Al-LDHs.

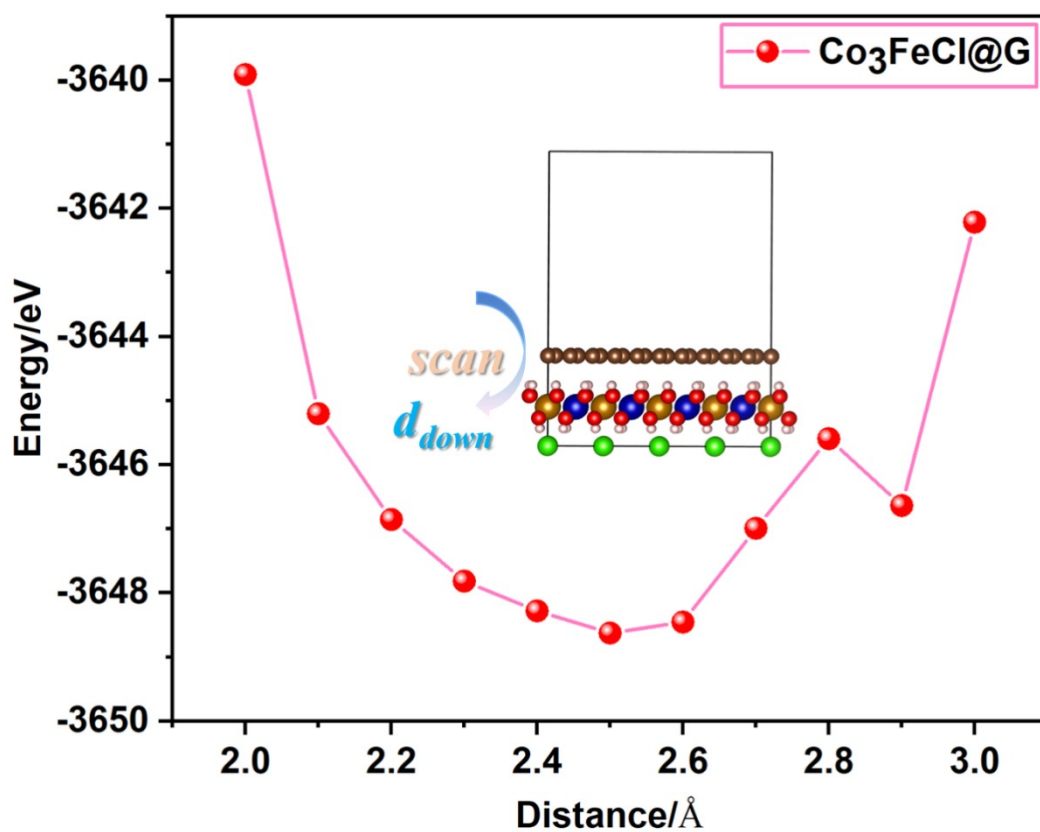


Figure S5. Potential energy surface scans for heterobilayer graphene/ $\text{Co}_3\text{Fe-LDH}$ s systems are performed based on the distance between graphene and $\text{Co}_3\text{Fe-LDH}$ s.

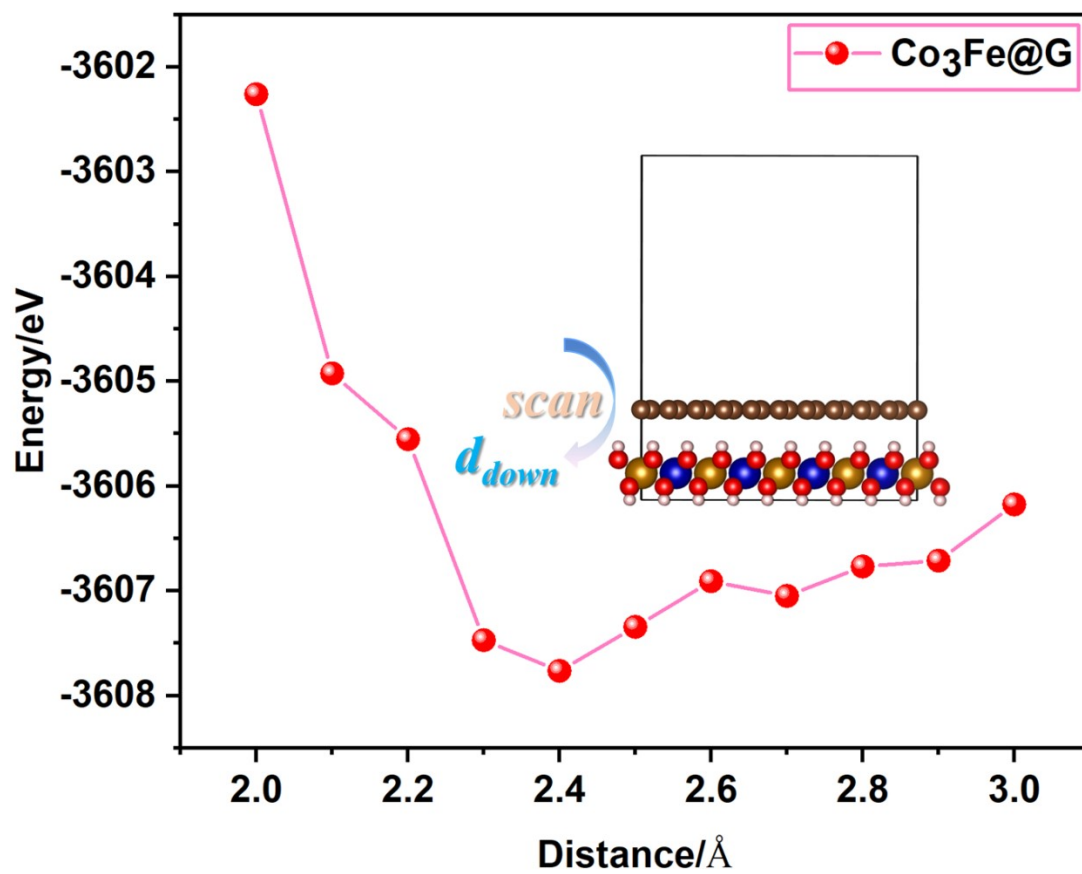


Figure S6. Potential energy surface scans for heterobilayer graphene/ Co_3Fe -LDHs systems are performed based on the distance between graphene and Co_3Fe -LDHs.

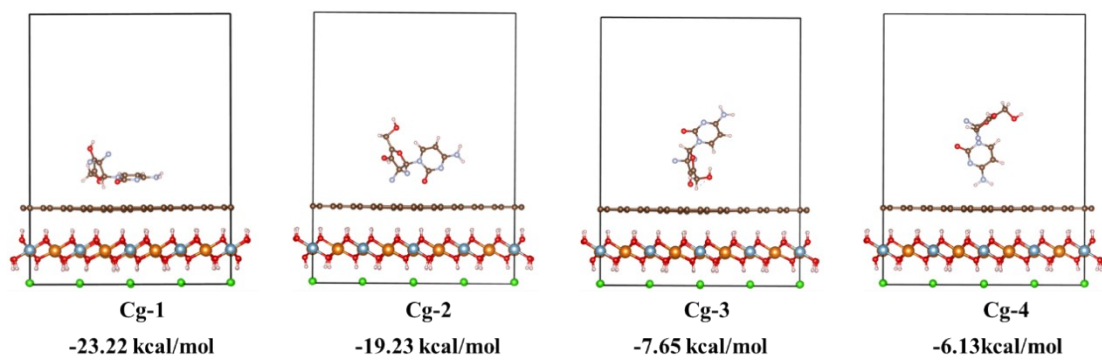


Figure S7. Different adsorption configurations for gemcitabine on heterobilayer graphene/Mg₃Al-LDHs.

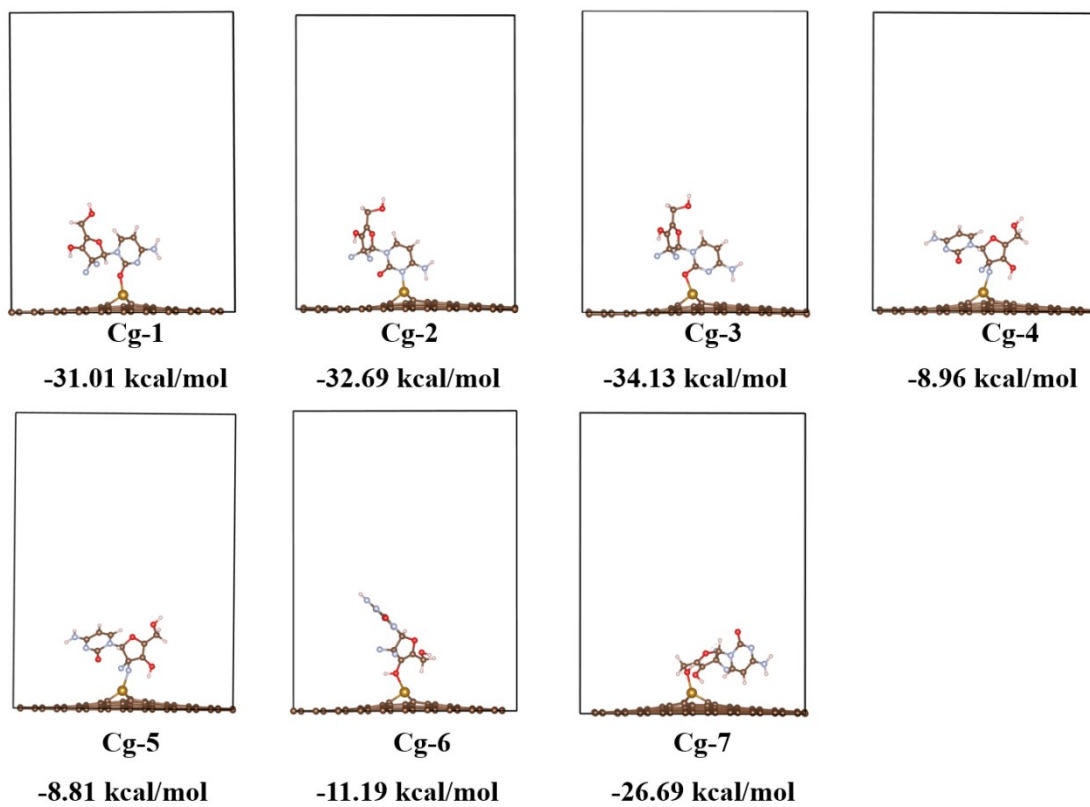
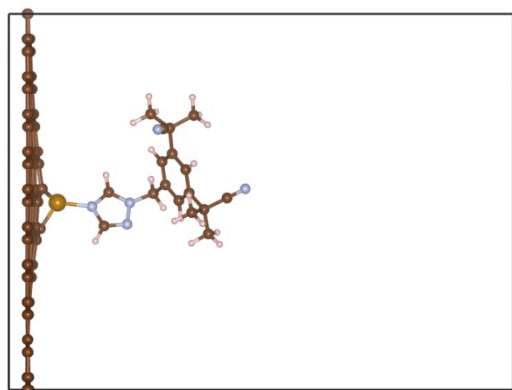
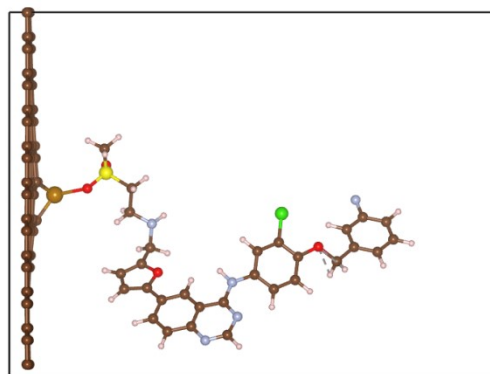


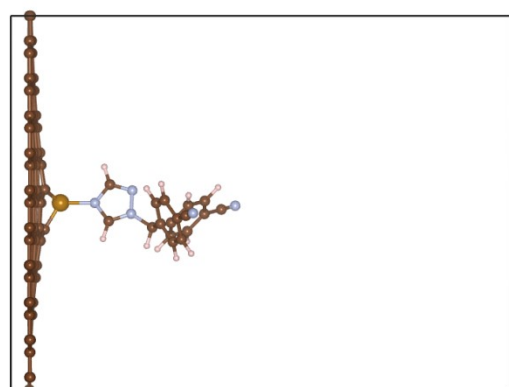
Figure S8. Different adsorption configurations for gemcitabine on Fe doped graphene.



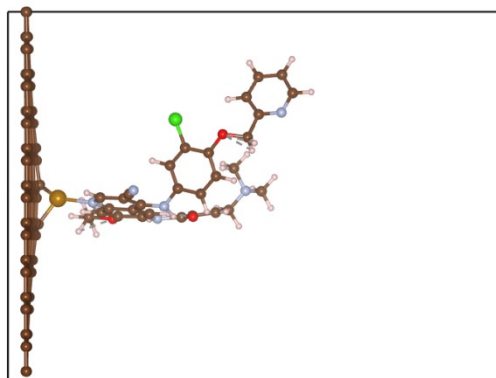
Fe-anastrozole



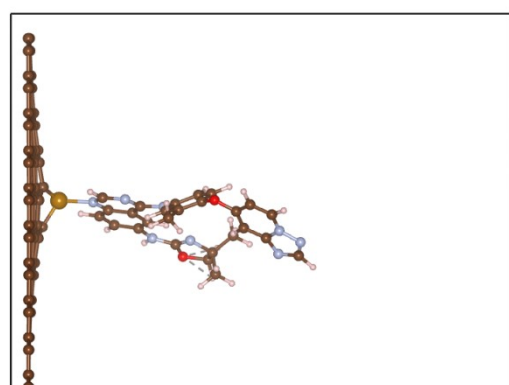
Fe-lapatinib



Fe-letrozole



Fe-neratinib



Fe-tucatinib

Figure S9. Different adsorption configurations for different potential breast drugs on Fe doped graphene.

Table S1. Lattice mismatch and strain values of graphene/M₃N-LDH heterobilayers.

System	L_G Å	L_{LDH} Å	Matched L Å	Lattice mismatch %	Graphene strain %	LDH strain %
Graphene/Ca ₃ Al-LDH	24.60	24.56	24.58	0.16	-0.08	+0.08
Graphene/Mg ₃ Al-LDH	24.60	24.40	24.50	0.82	-0.41	+0.41
Graphene/Ni ₃ Al-LDH	24.60	24.48	24.54	0.49	-0.24	+0.25
Graphene/Zn ₃ Al-LDH	24.60	24.56	24.58	0.16	-0.08	+0.08
Graphene/Co ₃ Fe-LDH-Cl	24.60	25.04	24.82	1.77	+0.89	-0.88
Graphene/Co ₃ Fe-LDH	24.60	24.80	24.70	0.81	+0.41	-0.40

Positive and negative strain values indicate tensile and compressive strain, respectively.