Electronic Supplementary Material (ESI) for RSC Advances.
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Supporting Information

Systems	Frequencies	Vibrational Assignments
ZVD_Fe_Se@C_3N_4	3787,3776,3769	Asymmetric NH_2
	3649,3646	Asymmetric NH
	3634,3627,	Symmetric NH_2
	3508	Symmetric OH
	3224	Asymmetric CH_2
	3174,3152	Asymmetric CH_3
	3063	Symmetric CH_3
ZVD_Os_Se@C_3N_4	3921	Symmetric OH
	3786,3769	Asymmetric NH_2
	3656,3648,3644	Symmetric NH
	3634	Symmetric NH_2
	3232	Symmetric CH
	3176	Asymmetric CH_2

Iron group transition-metals (Fe, Ru, Os) coordination of Se-doped graphitic carbon (Se@g-C_3N_4) nanostructured for smart therapeutic delivery of Zidovudine (ZVD) as an antiretroviral drug: Perspective from theoretical calculations

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	3174,3141	Asymmetric CH_3
	3103,3063	Symmetric CH_2
	3054	Symmetric CH_3
ZVD_Ru_Se@C_3N_4	3938	Symmetric OH
	3792,3791,3758,	Asymmetric NH_2
	3658,3651	Symmetric NH
	3627	Symmetric NH_2
	3273	Symmetric CH
	3172,3147,	Asymmetric CH_3
	3058	Symmetric CH_3
	2283	Symmetric RuH
ZVD_Se@C_3N_4	3794,3789,3769,	Asymmetric NH_2
	3652	Symmetric NH
	3625	Symmetric NH_2
	3246,3199	Symmetric CH
	3169,3148,3058	Asymmetric CH_3

Table S1: Analysis of the vibrational stability

Table S2: Analysis of molecular dynamic simulations

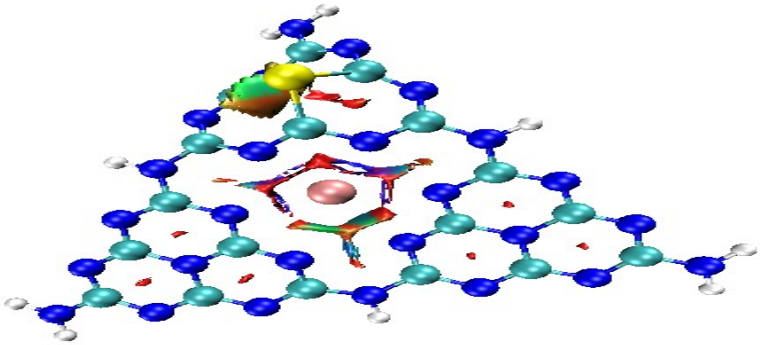
SURFACES					INTERACTIONS				
Fe_Se@C_3N_4					**ZVD_Fe_Se@C_3N_4**				
Parameters	Initial energy	Final energy	Average	Standard deviation	Parameters	Initial energy	Final energy	Average	Standard deviation
Tot. energy (kcal/mol)	1512.439	1511.881	1509.189	2.313	Tot. energy(kcal/mol)	2007.364	2013.267	2011.286	3.652
Pot. energy (kcal/mol)	1465.360	874.226	866.014	52.255	Pot. energy(kcal/mol)	1930.972	1158.973	1174.708	54.048
Kin. energy (kcal/mol)	47.079	637.655	643.176	51.334	Kin. energy(kcal/mol)	76.392	854.294	836.578	53.181
Temperature (K)	298.000	4036.233	4071.177	324.932	Temperature (K)	298.000	3332.539	3263.428	207.456
Os_Se@C_3N_4					**ZVD_Os_Se@C_3N_4**				
Tot. energy (kcal/mol)	1202.386	1198.556	1198.509	1.472	Tot. energy(kcal/mol)	1782.040	1769.695	1769.882	1.948
Pot. energy (kcal/mol)	1155.307	705.325	673.912	42.541	Pot. energy(kcal/mol)	1705.648	1013.405	976.022	50.573
Kin. energy (kcal/mol)	47.079	493.231	524.597	41.811	Kin. energy(kcal/mol)	76.392	756.289	793.860	49.647
Temperature (K)	298.000	3122.054	3320.596	264.658	Temperature (K)	298.000	2950.229	3096.789	193.668
Ru_Se@C_3N_4					**ZVD_Ru_Se@C_3N_4**				
Tot. energy (kcal/mol)	1192.250	1195.087	1188.994	2.004	Tot. energy(kcal/mol)	1485.699	1480.201	1479.898	1.513
Pot. energy (kcal/mol)	1145.172	635.836	669.339	41.739	Pot. energy(kcal/mol)	1409.307	825.112	827.883	42.890
Kin. energy (kcal/mol)	47.079	559.250	519.656	41.035	Kin. energy(kcal/mol)	76.392	655.089	652.015	42.127
Temperature (K)	298.000	3539.946	3289.319	259.746	Temperature (K)	298.000	2555.454	2543.461	164.334
Se@C_3N_4					**ZVD_Se@C_3N_4**				
Tot. energy (kcal/mol)	1174.597	1168.741	1169.609	1.443	Tot. energy(kcal/mol)	1590.769	1589.190	1585.483	2.322
Pot. energy (kcal/mol)	1128.406	593.919	655.530	41.357	Pot. energy(kcal/mol)	1515.265	911.966	869.428	47.621
Kin. energy (kcal/mol)	46.191	574.822	514.080	40.650	Kin. energy(kcal/mol)	75.504	677.224	716.055	46.752
Temperature (K)	298.000	3708.484	3316.603	262.258	Temperature (K)	298.000	2672.882	2826.142	184.523

Table S3: EDA analysis

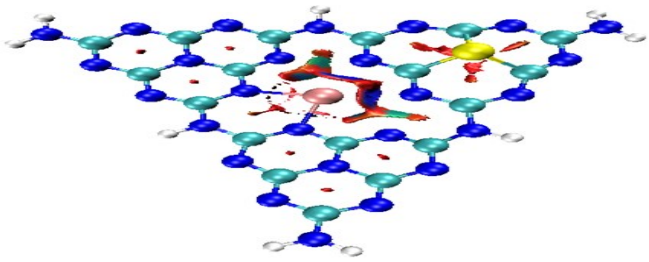
Complexes	ΔE_{tot} (kj/mol)	ΔE_{orb} (kj/mol)	ΔE_{steric} (kj/mol)
ZVD_Fe_Se@C_3N_4	-787.7	-19691.3	18903.6
ZVD_Os_Se@C_3N_4	-1837.9	-5776.1	3938.2
ZVD_Ru_Se@C_3N_4	-787.7	-9714.4	8926.7
ZVD_Se@C_3N_4	-262.6	-3150.6	2888

Table S4: Analysis of bond dissociation energies

Complexes	Energies	Before interaction	After interaction
ZVD_ Fe_Se@C_3N_4	**ΔH(hartrees)**	-5777.232549	-6740.058495
	Cv (cal/mol-kelvin)	137.377	201.400
	S (cal/mol-kelvin)	214.109	276.147
ZVD_Os_Se@C_3N_4	**ΔH(hartrees)**	-4604.340701	-5567.187842
	Cv (cal/mol-kelvin)	134.114	201.205
	S (cal/mol-kelvin)	202.932	276.115
ZVD_Ru_Se@C_3N_4	**ΔH(hartrees)**	-4608.548304	-5571.410260
	Cv (cal/mol-kelvin)	133.227	204.169
	S (cal/mol-kelvin)	201.157	289.246
ZVD_Se@C_3N_4	**ΔH(hartrees)**	-4513.632166	-5476.471072
	Cv (cal/mol-kelvin)	129.102	196.309
	S (cal/mol-kelvin)	200.751	281.757



Fe_Se@C_3N_4



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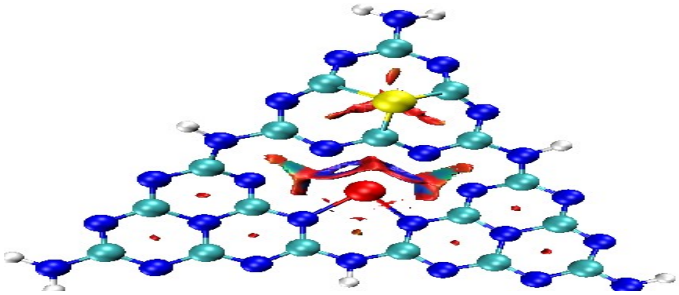

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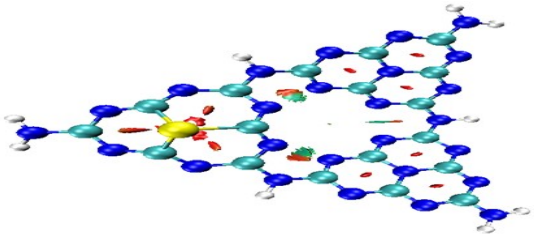

Se@C_3N_4

FIG. S1: Plots demonstrating the QTAIM of the studied adsorbents

Table S5: frequency scaling factors for interactions

Systems	Frequency scaling factors (cm^{-1})
ZVD_Fe_Se@C_3N_4	1.00
ZVD_Os_Se@C_3N_4	1.00
ZVD_Ru_Se@C_3N_4	1.00
ZVD_Se@C_3N_4	1.00

$Fe\_Se@C_3N_4$

BCPs: 105

Eigenvalues of Hessian: 0.8068238083E-01 -0.1240909796E-01 -0.1439806657E-01

BCPs: 86

Eigenvalues of Hessian: -0.7658421793E-02 -0.8167437063E-02 0.4870697019E-01

$Os\_Se@C_3$

BCPs: 85

Eigenvalues of Hessian: 0.3568443039E-02 0.1193430711E+00 -0.1819774842E-01

BCPs: 112

Eigenvalues of Hessian: -0.3179864756E-02 0.1206931094E+00 -0.1821569506E-01

$Ru\_Se@C_3N_4$

BCPs: 103

Eigenvalues of Hessian: 0.2943606577E+00 -0.4926281633E-01 -0.3524488154E-01

BCPs: 85

Eigenvalues of Hessian: -0.6811063517E+00 0.7404284668E+00 -0.6078778218E+00

$Se@C_3N_4$

BCPs: 95

Eigenvalues of Hessian: 0.2556798421E+00 -0.1313657293E+00 -0.1218438588E+00

BCPs: 107

Eigenvalues of Hessian: 0.1158982737E+00 -0.1599473872E-01 -0.1562365172E-01

Fig S2: evidence of λ1, λ2 and λ3 values from Multiwfn files

Table S6: Calculated energy gaps of surfaces and interactions using PBEO hybrid density functional

SYSTEMS	**ENERGY GAP(eV)**
$Fe\_Se@C_3N_4$	1.239
$Os\_Se@C_3N_4$	1.082
$Ru\_Se@C_3N_4$	1.073
$Se@C_3N_4$	1.663
$ZVD\_Fe\_Se@C_3N_4$	0.240
$ZVD\_Os\_Se@C_3N_4$	0.485
$ZVD\_Ru\_Se@C_3N_4$	0.695
$ZVD\_Se@C_3N_4$	-0.024

ZVD_Fe_Se@C_3N_4

BCPs: 114

Eigenvalues of Hessian: -0.9596185631E-02 -0.1361456106E-01 0.7429645141E-01

BCPs: 166

Eigenvalues of Hessian: -0.6975879367E-03 0.3410287131E-02 0.2022223172E-01

ZVD_Os_Se@C_3

BCPs: 8

Eigenvalues of Hessian: -0.3836610501E+06 -0.3836489828E+06 -0.3836547221E+06

BCPs: 6

Eigenvalues of Hessian: -0.1704919976E+06 -0.1704929079E+06 -0.1704906517E+06

ZVD_Ru_Se@C_3

BCPs: 170

Eigenvalues of Hessian: -0.2188668519E+00 -0.2077106109E+00 0.6754240322E+00

BCPs: 210

Eigenvalues of Hessian: -0.1246828421E+01 0.1055167227E+01 -0.1215626750E+01

ZVD_Se@C_3N_4

BCPs: 25

Eigenvalues of Hessian: -0.5434233795E+01 -0.6036895092E+01 -0.6032582367E+01

BCPs: 27

Eigenvalues of Hessian: -0.1701352465E+06 -0.1701359129E+06 -0.1701374020E+06