Supplementary information

Performance and mechanisms of waste-based carbon adsorbents in heavy metal removal- an experimental and theoretical approach

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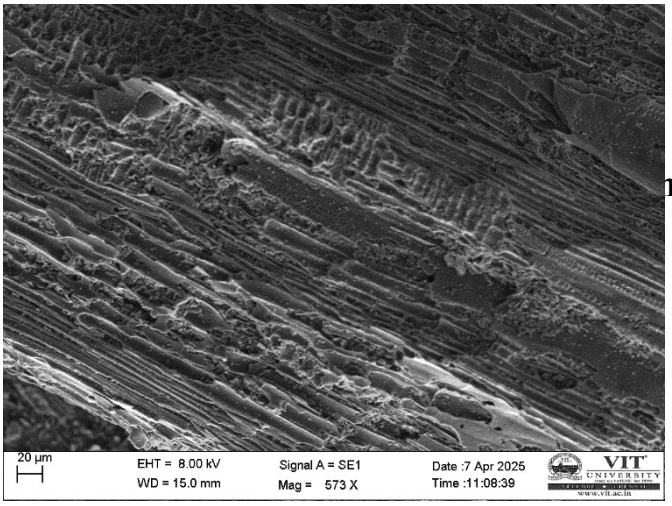
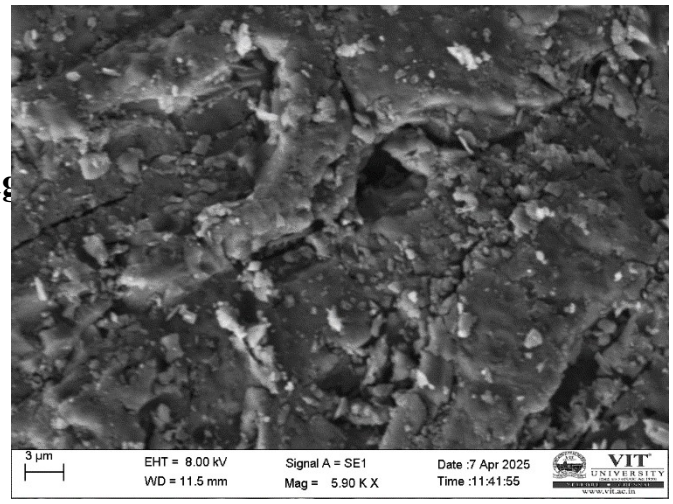
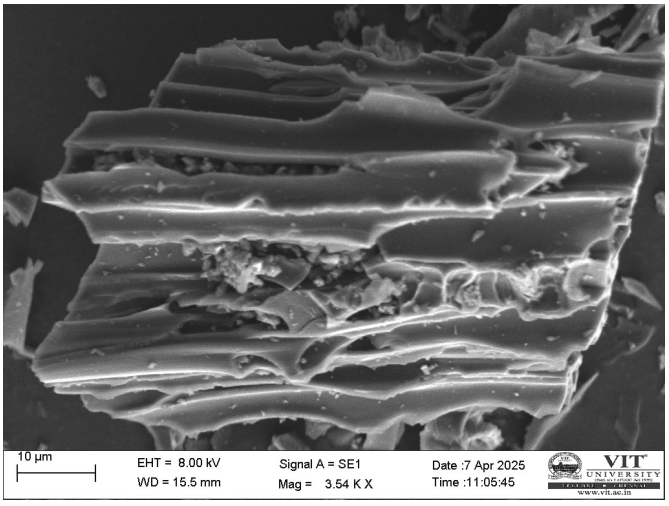
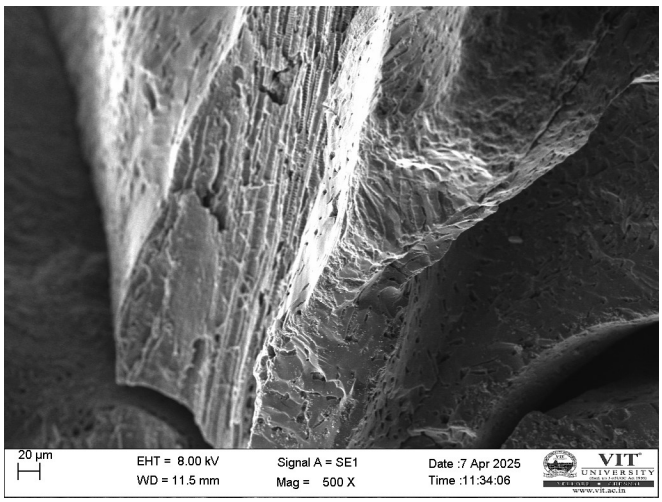
Outline

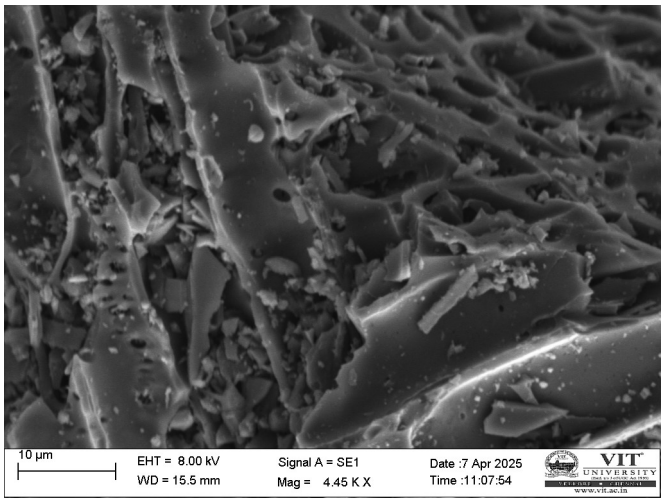
S1 - Additional SEM Images of all selected materials

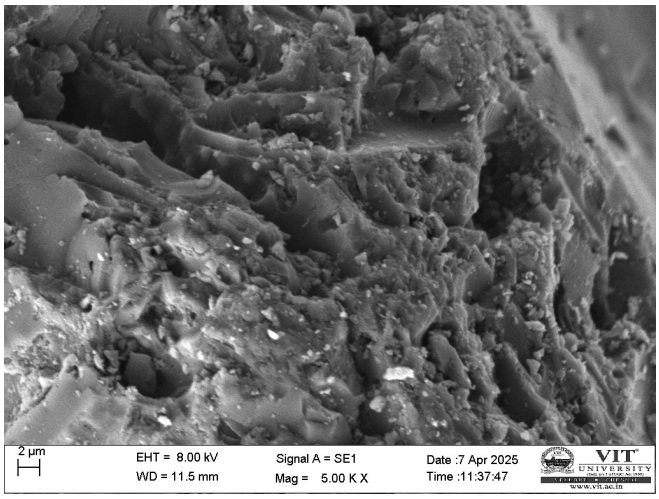






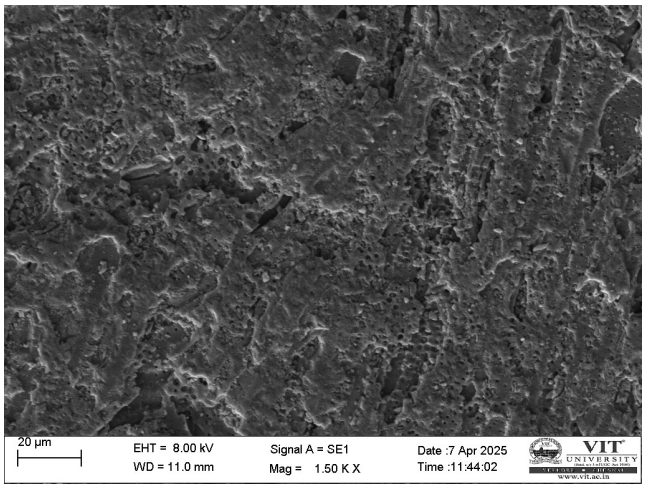


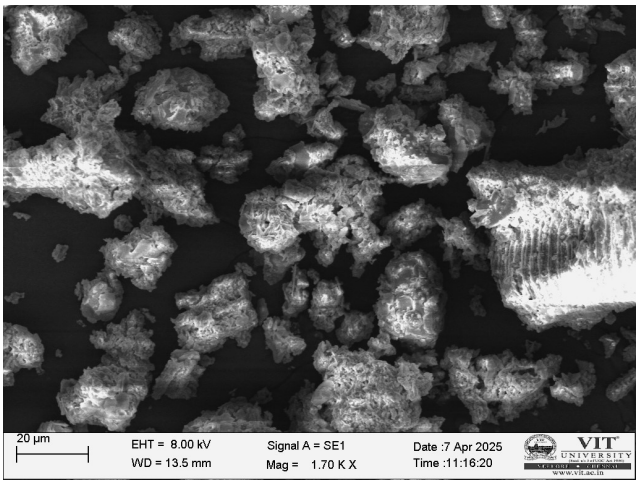


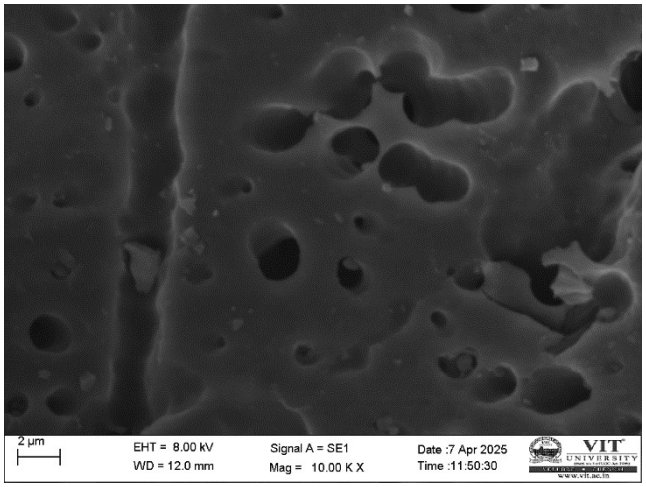


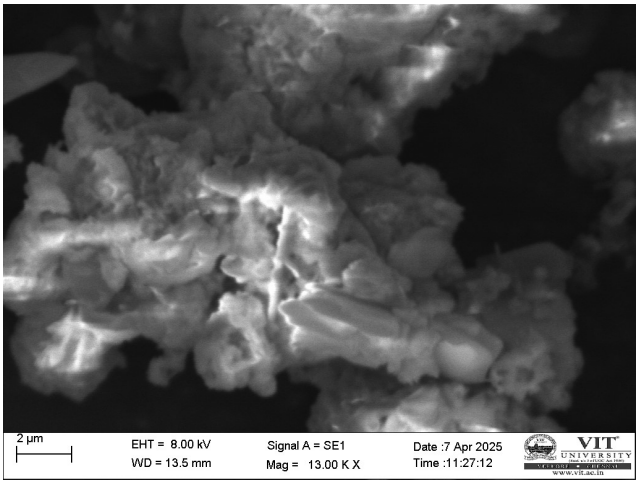
Proposis Julifolra Biochar

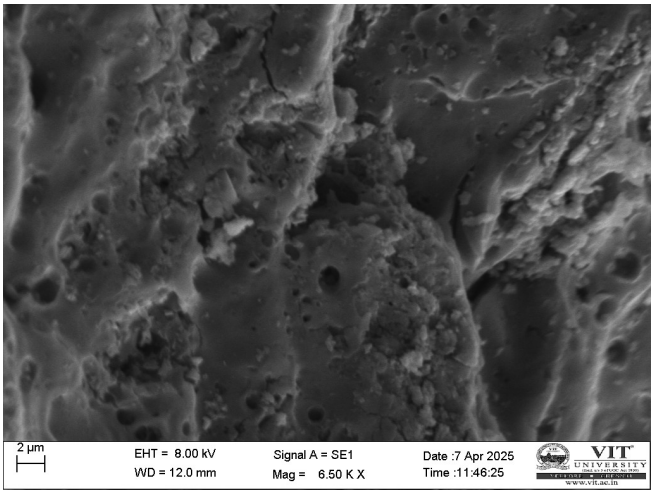
GAC

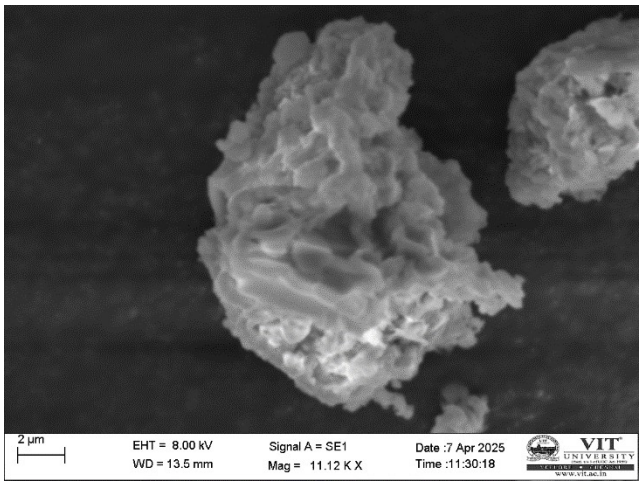










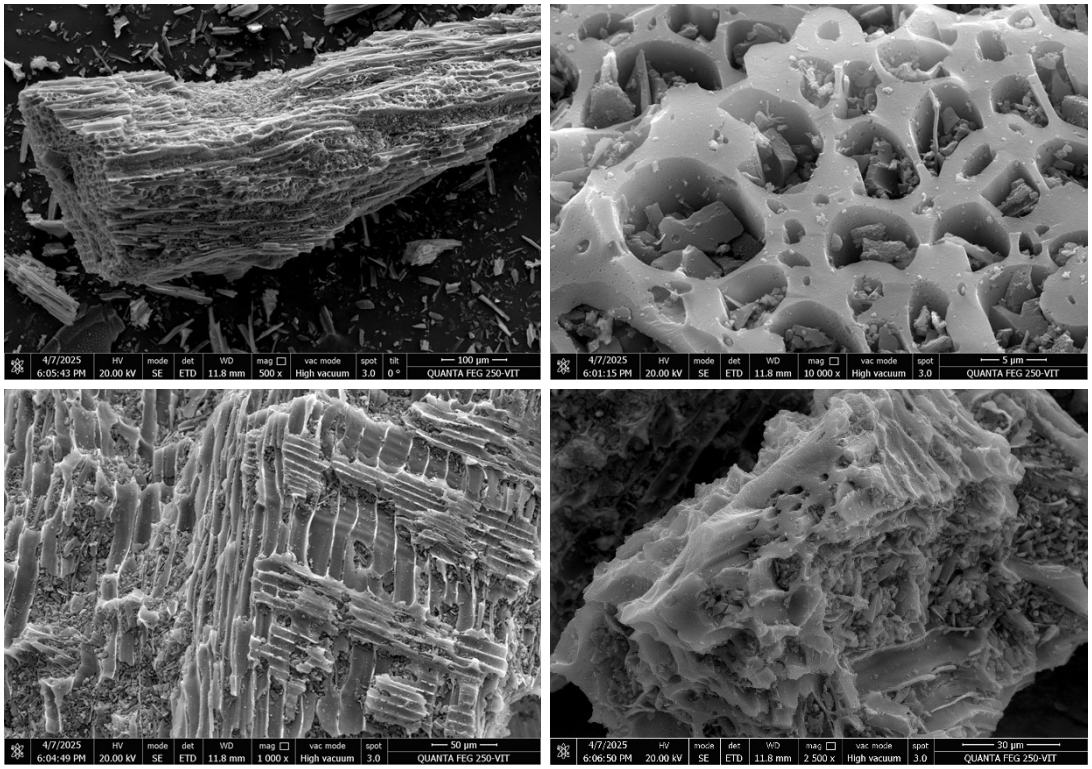


GAC - CS

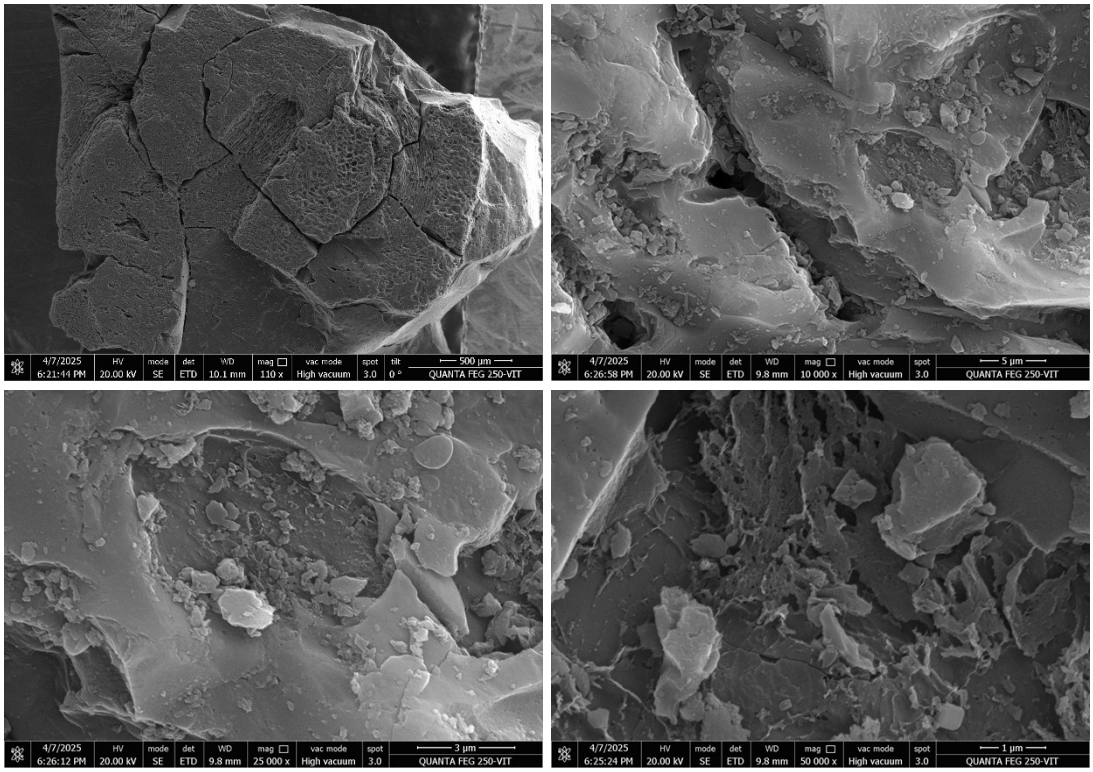
BN Char

S1 - Additional SEM images of all selected materials

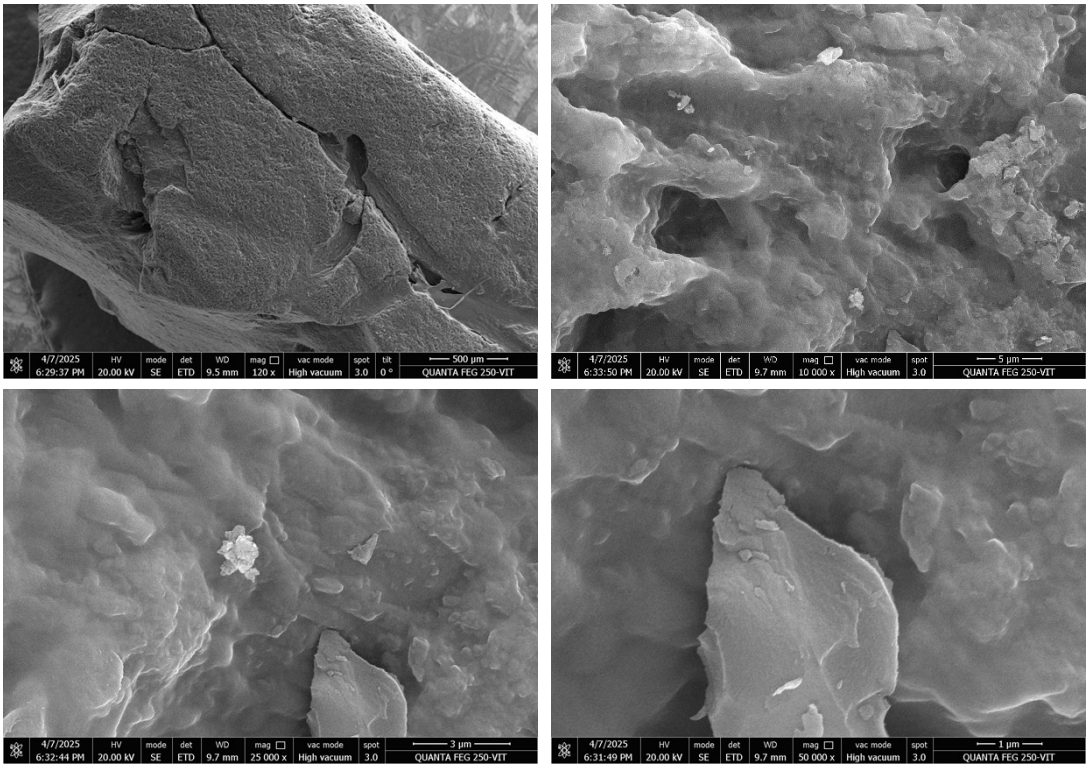
S2 - Additional FE - SEM Images of all selected materials



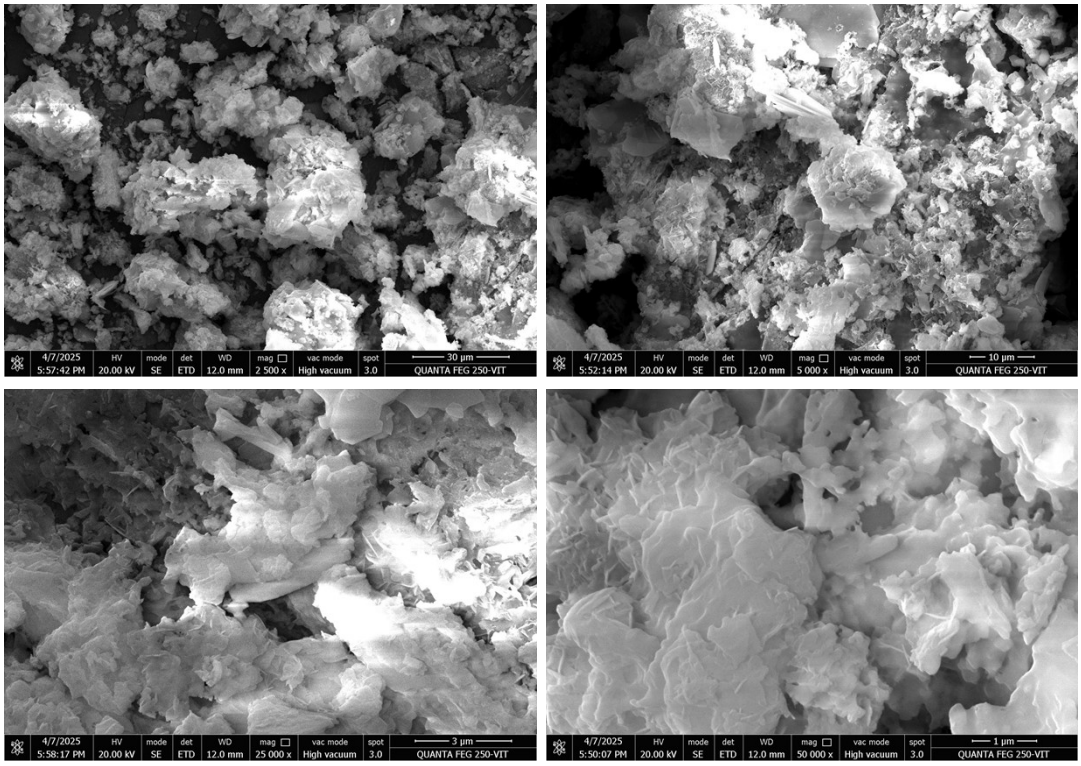
Proposis Julifolra Biochar



GAC



GAC - CS



BN Char

Fig S2 – Additional FE-SEM images of all selected materials

S3 - EDX Spectral images of chars

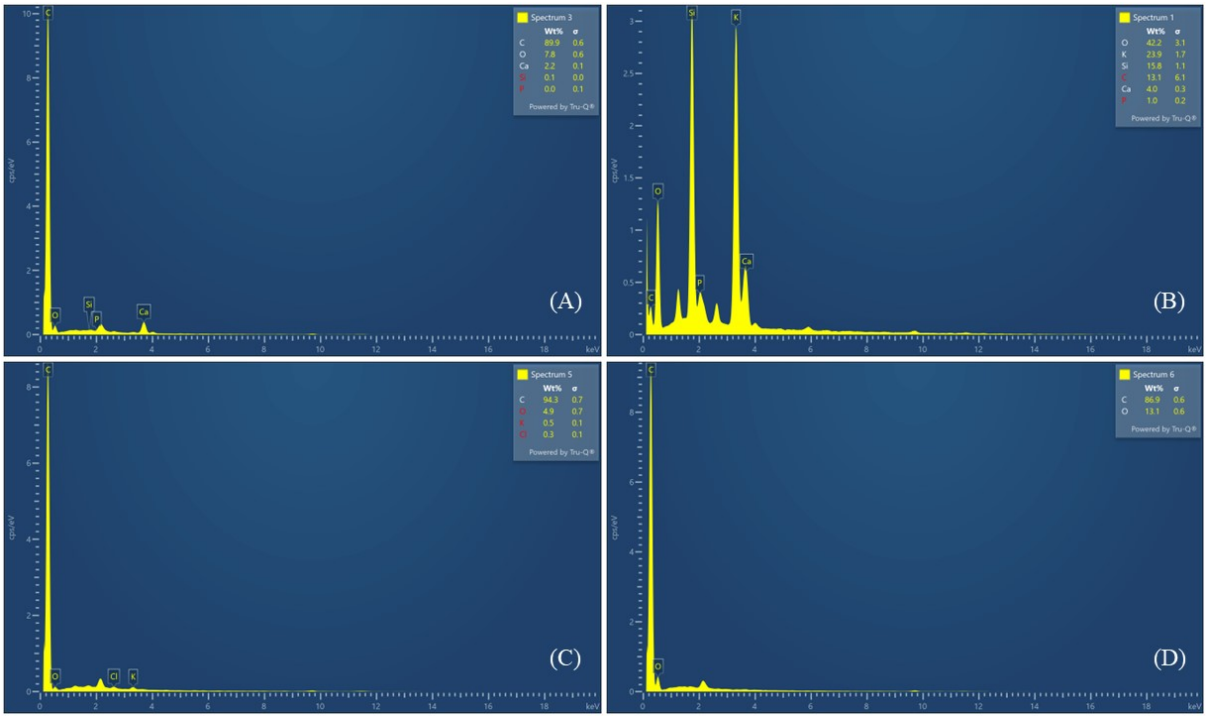
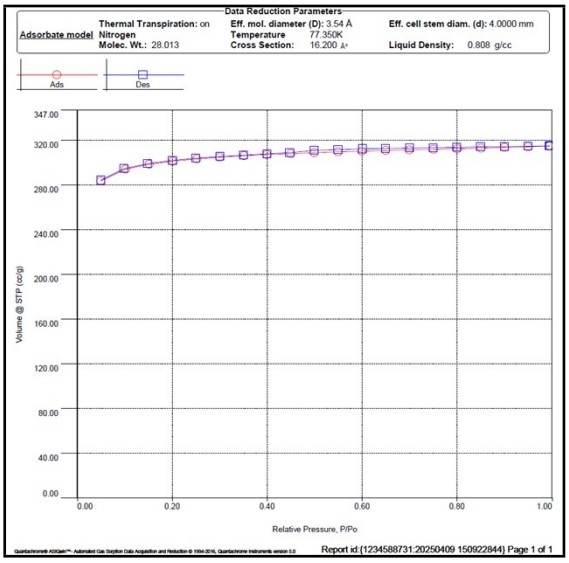
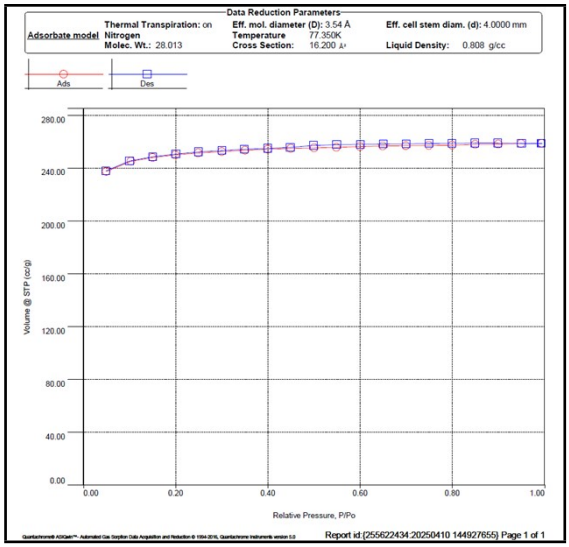


Fig S3 - EDX images of (A) PJBC, (B) BN Char, (C) GAC, and (D) GAC-CS.

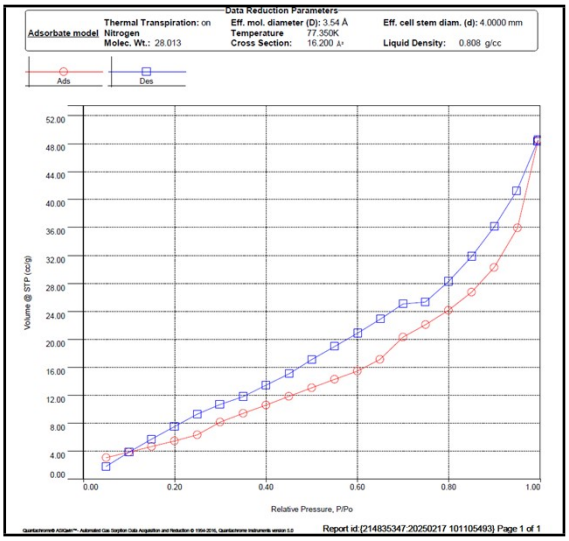
S4 - Original BET Instrument Output



(A)



(B)



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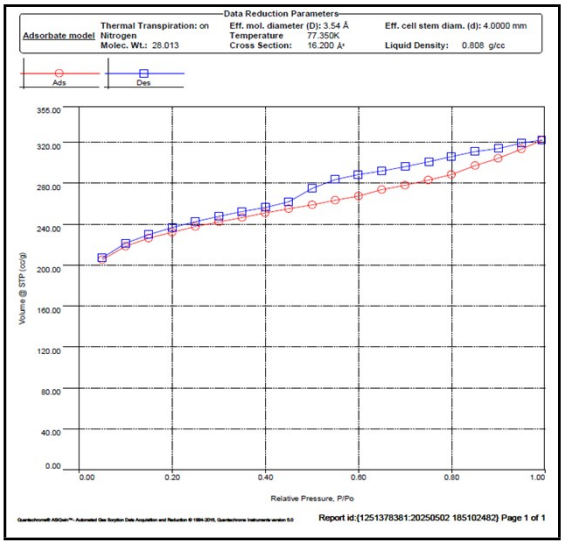
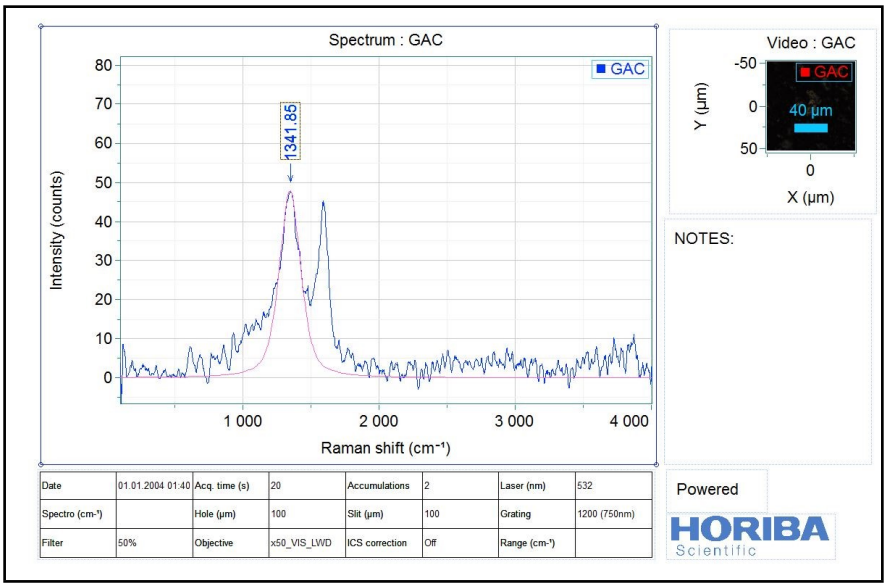


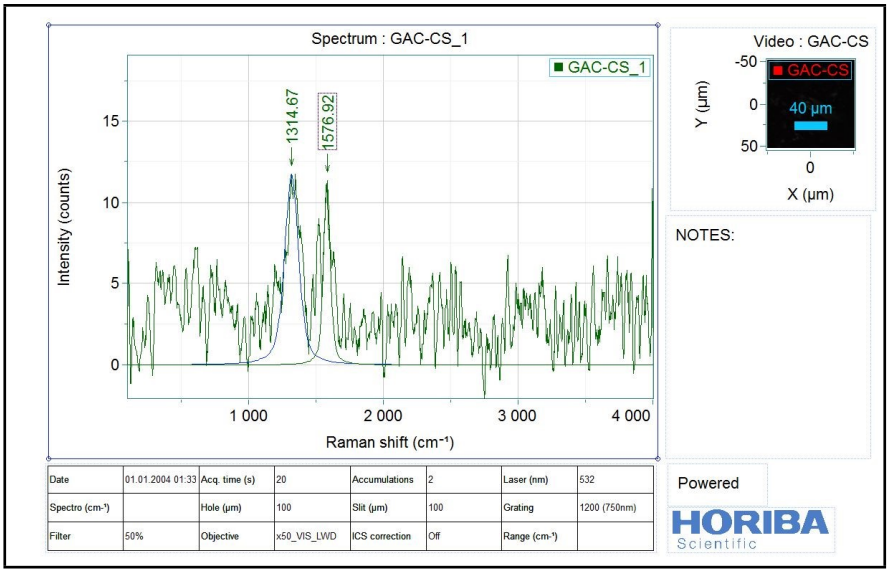
(D)

Fig S4 – BET original output of (A) GAC, (B) GAC-CS, (C) BN Char and (D) PJ Biochar

S5 - Original Raman Instrument Output



(A)



(B)

Fig S5 – BET original output of (A) GAC, (B) GAC-CS.

S6 – Co-ordinates of selected molecules for this study

Non functionalized graphite like molecule (G)

C	-0.12172000	-1.43742900	-0.03947800
C	-1.33494700	-0.65049200	-0.02739400
C	-1.27553100	0.75364100	-0.06602600
C	0.05226800	1.40848100	-0.33876600
C	1.20632700	0.67189500	0.32855100
C	1.14172800	-0.81876700	0.10269500
C	2.29801400	-1.58367000	0.16982600
C	2.51638000	1.32424300	-0.07808700
C	0.11115300	2.88882900	-0.02164300
C	-2.43623800	1.52212100	0.01776500
C	-2.59749200	-1.30056100	0.00832200
C	-0.20889500	-2.85151400	-0.10184300
C	-1.50285400	-3.47025800	-0.13039200
C	-2.64268900	-2.73080600	-0.05290900
C	0.98298500	-3.60612500	-0.08228800
C	2.20722700	-2.98372900	0.04656300
C	3.61640900	-0.88954500	0.41449800
C	3.69618000	0.43555500	-0.35746300
C	2.54078200	2.67113400	-0.14863500
C	1.34008200	3.46276000	0.04480000
C	-1.13263400	3.60948900	0.06920400
C	-2.32807900	2.97387000	0.05035500
C	-3.68632400	0.86586400	0.09979400
C	-3.76539100	-0.50928300	0.07553300
H	3.70577500	0.19853000	-1.43008600
H	4.63157300	0.95956800	-0.14299500

H	3.72761900	-0.68986200	1.48860200
H	4.44505500	-1.54317200	0.13109100
H	1.10150000	0.82967900	1.42034700
H	3.47287100	3.18632000	-0.36094900
H	1.43091800	4.53549200	0.18191400
H	3.11547400	-3.57667500	0.07519600
H	0.92354900	-4.68705900	-0.14894900
H	-1.55459700	-4.55220500	-0.18703300
H	-3.61211500	-3.21730300	-0.04556100
H	-4.73156300	-1.00094700	0.10791900
H	-4.59040200	1.46164700	0.16596500
H	-3.24758000	3.54598700	0.11337200
H	-1.09142900	4.68963500	0.16674100
H	0.21289800	1.32616800	-1.43347200

Graphite functionalised with hydroxyl group (G+OH)

C	-0.49817200	1.42866600	-0.00387400
C	-1.47503300	0.36478400	-0.03042900
C	-1.07628800	-0.98285800	-0.02352300
C	0.36741200	-1.30394300	0.27766500
C	1.29664500	-0.28448100	-0.38551500
C	0.87781200	1.14296700	-0.14634300
C	1.80882100	2.16928000	-0.20799200
C	2.74524900	-0.60204000	-0.08869400
C	0.78482400	-2.70877600	-0.13709300
C	-2.00919700	-2.01286500	-0.13020200
C	-2.85956500	0.68332100	-0.06253200
C	-0.93281100	2.77496500	0.07638800
C	-2.33935000	3.05418800	0.11185200
C	-3.25942900	2.05605100	0.02162400
C	0.03534600	3.80127200	0.06853900

C	1.37440900	3.50232900	-0.06911400
C	3.25701500	1.83541100	-0.47548000
C	3.66978900	0.53612400	0.22820300
C	3.10417800	-1.90227200	-0.09048900
C	2.11642800	-2.95291400	-0.25905700
C	-0.24046800	-3.71578600	-0.23368800
C	-1.55324700	-3.39267500	-0.19840500
C	-3.38176300	-1.68295500	-0.20649000
C	-3.79524800	-0.37009400	-0.15227200
H	3.62259400	0.71426600	1.31221800
H	4.70417000	0.26990500	-0.00497400
H	3.40977300	1.72509400	-1.55732300
H	3.89897300	2.65877200	-0.15261600
H	1.16917600	-0.46702800	-1.47022000
H	4.14262600	-2.18369900	0.05386800
H	2.45944600	-3.96721600	-0.43893700
H	2.10783200	4.30163200	-0.09199300
H	-0.28913200	4.83294700	0.15020600
H	-2.65751000	4.08852100	0.18475400
H	-4.31951100	2.28555400	0.01983800
H	-4.85275300	-0.13060100	-0.18021500
H	-4.11180500	-2.48069900	-0.29064600
H	-2.30674000	-4.16951500	-0.27045900
H	0.06642800	-4.74977100	-0.35383000
O	0.44412100	-1.22148700	1.72524900
H	1.29933800	-1.58245900	1.98985700

Graphite functionalised with carboxylic group (G+COOH)

C	1.52576700	0.56976500	-0.10221800
C	0.44250200	1.52664700	-0.15741500
C	-0.89629300	1.10211000	-0.22817400

C	-1.20025400	-0.36750700	0.01922300
C	-0.12695600	-1.24788500	-0.62186600
C	1.27891900	-0.80588600	-0.30326400
C	2.32538200	-1.71401100	-0.33483300
C	-0.43003900	-2.71349400	-0.37523500
C	-2.57058400	-0.79984500	-0.50824400
C	-1.93548300	2.01429200	-0.40424600
C	0.73310100	2.91830200	-0.14862900
C	2.85572400	1.03030500	0.06024200
C	3.10108800	2.44092400	0.14676200
C	2.09045400	3.34310300	0.02132200
C	3.90234300	0.08430900	0.07717600
C	3.63904100	-1.25567300	-0.11353600
C	2.03419400	-3.16502700	-0.63539600
C	0.70909000	-3.61045600	-0.00095300
C	-1.71684900	-3.09903300	-0.47281600
C	-2.77127800	-2.12746800	-0.70246000
C	-3.57901500	0.21247100	-0.69158500
C	-3.29452100	1.53008500	-0.60066800
C	-1.62877600	3.39303100	-0.44193900
C	-0.33193900	3.83352200	-0.28951600
H	0.82033700	-3.54984600	1.08978800
H	0.48119400	-4.65030500	-0.24908300
H	1.98495400	-3.30945100	-1.72289800
H	2.85285400	-3.79283400	-0.27487800
H	-0.25690300	-1.09249700	-1.70933200
H	-1.98514100	-4.14489800	-0.36353200
H	-3.75342600	-2.47758400	-1.00429900
H	4.45373500	-1.97231000	-0.11095000
H	4.92112400	0.42696300	0.22169300
H	4.12288300	2.77821100	0.28313400
H	2.29735600	4.40731600	0.05318300

H	-0.11441900	4.89606500	-0.28477700
H	-2.43394200	4.10686400	-0.57786500
H	-4.07717400	2.26781500	-0.73884200
H	-4.58649400	-0.11489700	-0.92646500
C	-1.18048400	-0.56302700	1.55792600
O	-0.34907100	-1.17898800	2.17436900
O	-2.20973200	0.06911000	2.16332700
H	-2.10732200	-0.07691200	3.11560300

Graphite functionalised with Amino group (G+NH_2)

C	-0.52907800	1.41940400	-0.00702800
C	-1.48251000	0.33465300	-0.03571800
C	-1.05172900	-1.00399600	-0.02070200
C	0.40185600	-1.29288400	0.29329700
C	1.29947400	-0.25604600	-0.38665900
C	0.85312500	1.16219000	-0.14394600
C	1.76164500	2.20813600	-0.20079700
C	2.75787300	-0.54433900	-0.09933400
C	0.84782100	-2.68532000	-0.15431300
C	-1.96298700	-2.05407100	-0.12689900
C	-2.87353000	0.62204800	-0.07439900
C	-0.99329600	2.75548700	0.06955900
C	-2.40574700	3.00379100	0.09749300
C	-3.30387100	1.98593200	0.00428000
C	-0.04758800	3.80299200	0.06594400
C	1.29787800	3.53203600	-0.06421700
C	3.21917900	1.90709800	-0.45797700
C	3.65373800	0.61012600	0.23755100
C	3.14737600	-1.83505900	-0.13396200
C	2.18053700	-2.90324800	-0.30935200
C	-0.15497400	-3.71702600	-0.24083800

C	-1.47541700	-3.42529600	-0.19018900
C	-3.34344100	-1.75539900	-0.20807200
C	-3.78625700	-0.45215600	-0.16230400
H	3.59044600	0.77682100	1.32261000
H	4.69619300	0.36931900	0.01257300
H	3.38437600	1.81077300	-1.53932200
H	3.84013400	2.74112100	-0.12122100
H	1.16820200	-0.43981100	-1.47007900
H	4.19329300	-2.09501700	-0.00271600
H	2.54012500	-3.90803400	-0.50945500
H	2.01447400	4.34665300	-0.08288600
H	-0.39456100	4.82755400	0.14498600
H	-2.74683300	4.03114000	0.16645200
H	-4.36867300	2.19241700	-0.00387700
H	-4.84866600	-0.23609100	-0.19522600
H	-4.05473100	-2.56996800	-0.29279300
H	-2.21161000	-4.21932000	-0.25516300
H	0.17339400	-4.74432600	-0.36399600
N	0.52774000	-1.16312600	1.77144400
H	-0.16967700	-1.75104900	2.21733600
H	1.43947300	-1.50459400	2.06417300

Graphite functionalised with Methoxy group (G+OCH_3)

C	-1.33296400	0.88462800	-0.02630100
C	-1.50803700	-0.54773900	-0.09255000
C	-0.39971100	-1.41168100	-0.14795700
C	0.96860500	-0.83533900	0.14460100
C	1.09725500	0.54214000	-0.51684200
C	-0.05421600	1.45967700	-0.20807500
C	0.09932700	2.83672100	-0.26954900
C	2.48118100	1.13008300	-0.38332200

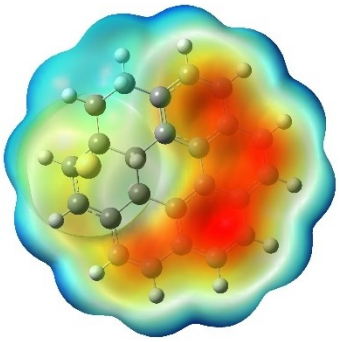
C	2.10724300	-1.72325700	-0.33250200
C	-0.56192200	-2.79110100	-0.25916400
C	-2.81939800	-1.09479900	-0.08980600
C	-2.46611300	1.72268800	0.11829300
C	-3.76989900	1.12890700	0.18623600
C	-3.93964500	-0.21539700	0.06182300
C	-2.27680800	3.12116100	0.13219000
C	-1.02345200	3.66263200	-0.06077700
C	1.44110700	3.41828000	-0.64865200
C	2.60641000	2.59579100	-0.08538700
C	3.52205100	0.28195200	-0.50524700
C	3.30985500	-1.14799000	-0.60025700
C	1.86360000	-3.14365000	-0.39601800
C	0.61033500	-3.64839200	-0.34024700
C	-1.87247000	-3.31998200	-0.30475300
C	-2.97033200	-2.49418400	-0.20483800
H	2.60363600	2.71814800	1.00727100
H	3.56706500	2.97875100	-0.43966500
H	1.51662300	3.44726900	-1.74389400
H	1.51317500	4.45370600	-0.30600400
H	1.00081300	0.29446700	-1.59219600
H	4.54050900	0.65707200	-0.48771400
H	4.15343100	-1.78247500	-0.85682900
H	-0.89681200	4.74013800	-0.07957900
H	-3.13695600	3.76817300	0.26604400
H	-4.62763600	1.78120600	0.30963200
H	-4.93452400	-0.64694300	0.08490100
H	-3.97020400	-2.91460800	-0.20845600
H	-2.00493500	-4.39257200	-0.39740800
H	0.45024200	-4.71930600	-0.40280500
H	2.71419200	-3.80417900	-0.53156600
O	0.93437700	-0.79770200	1.59580000

C	2.05797800	-0.33443900	2.32688700
H	2.18295900	0.74889800	2.23031300
H	1.84868800	-0.57559000	3.36995400
H	2.98485700	-0.83080100	2.02488000

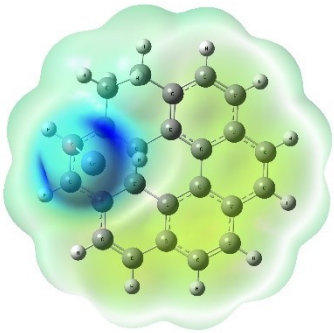
S7 - Calculated Energetic, Electronic, and Thermodynamic Parameters of the Complexes

Table S7. Total Energy (in Kcal/mol), Dipole moment (in Debye), Polarizability (in a.u.), Enthalpy (in Kcal/mol), Gibbs Free Energy (in Kcal/mol) and Entropy (in cal/mol-Kelvin) of the complexes

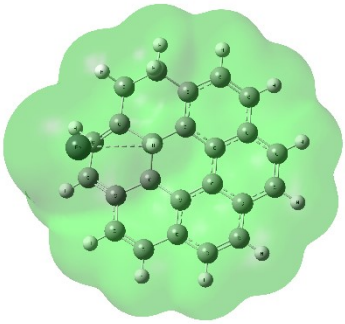
S.No	Complexes	Total energy (x 10^5 Kcal/mol)	Dipole moment (Debye)	Polarizability (a.u.)	Enthalpy (x 10^5 Kcal/mol)	Gibbs Free Energy (x 10^5 Kcal/mol)	Entropy (Cal/mol-kelvin)
1.	G	-5.80151	0.926	291.162	-5.79938	-5.79973	120.122
2.	G+NH_2	-6.14897	1.224	297.811	-6.14673	-6.14710	125.299
3.	G+OH	-6.27367	2.083	293.874	-6.27151	-6.27188	215.771
4.	G+COOH	-6.98520	0.659	303.608	-6.98296	-6.98336	303.608
5.	G+OCH_3	-6.52034	1.965	304.579	-6.51799	-6.51839	131.216
6.	G+Cd	-6.10326	0.969	343.325	-6.10111	-6.10153	141.965
7.	G+Cr	-6.34243	4.127	325.112	-6.34030	-6.34068	125.986
8.	G+Pb	-5.82321	2.854	365.078	-5.82107	-5.82147	134.514
9.	G+COOH+Cd	-7.28697	2.018	351.076	-7.28471	-7.28517	153.739
10.	G+OCH_3+Cd	-6.82212	3.179	349.202	-6.81976	-6.82021	151.203
11.	G+NH_2+Cd	-6.45076	2.493	345.894	-6.44849	-6.44892	143.517
12.	G+OH+Cd	-6.57545	2.825	339.969	-6.57327	-6.57370	143.921
13.	G+COOH+Cr	-7.52577	2.899	387.919	-7.52351	-7.52395	147.512
14.	G+OCH_3+Cr	-7.06138	3.66	328.839	-7.05903	-7.05944	136.518
15.	G+NH_2+cr	-6.68963	2.755	421.782	-6.68737	-6.68778	138.305
16.	G+OH+Cr	-6.81425	3.059	415.87	-6.81208	-6.81248	133.7
17.	G+COOH+Pb	-7.00674	1.684	367.588	-7.00450	-7.00495	151.973
18.	G+OCH_3+Pb	-6.54203	2.858	392.571	-6.53967	-6.54011	145.554
19.	G+NH_2+Pb	-6.17067	2.372	394.307	-6.16841	-6.16883	138.239
20.	G+OH+Pb	-6.29592	2.428	333.095	-6.29375	-6.29418	143.261



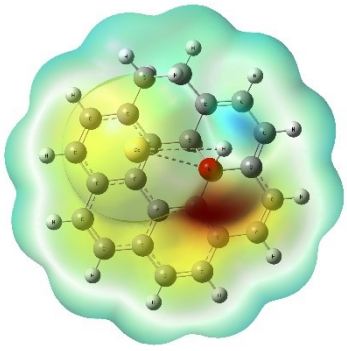
Graphite + Cd



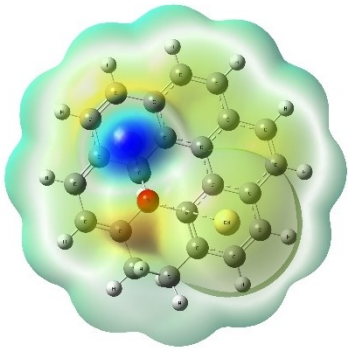
Graphite + Cr



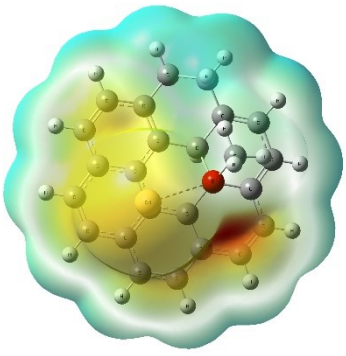
Graphite + Pb



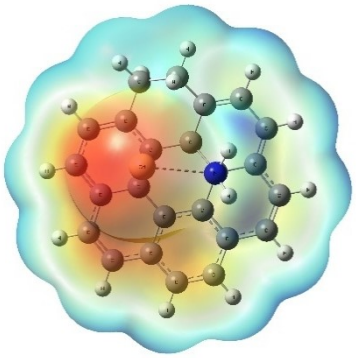
Graphite+ OH + Cd



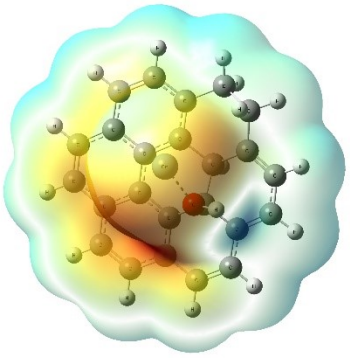
Graphite + COOH + Cd



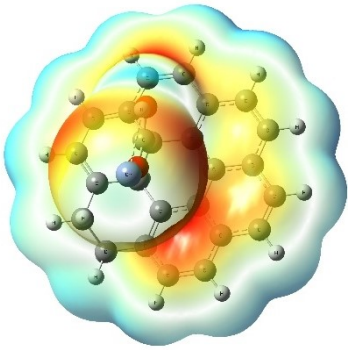
Graphite+ OCH_3 + Cd



Graphite + NH_2 + Cd

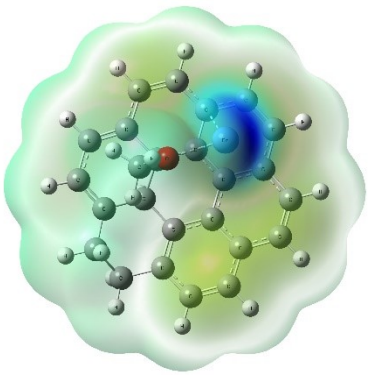


Graphite + OH + Cr

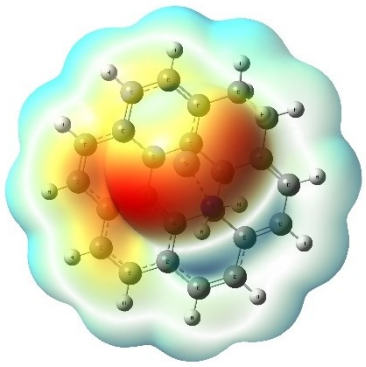


Graphite + COOH + Cr

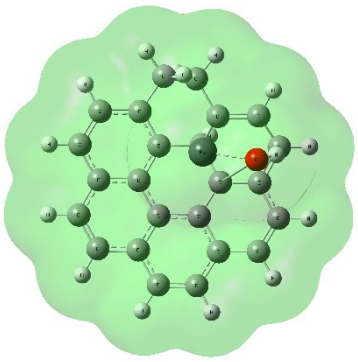
S8 – MEPs of all selected complexes



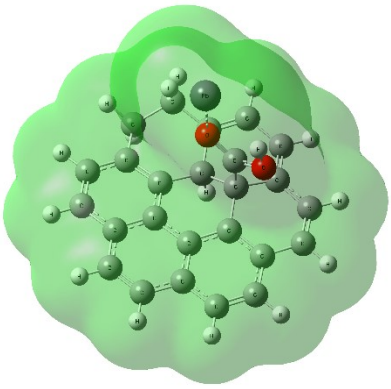
Graphite + OCH_3 + Cr



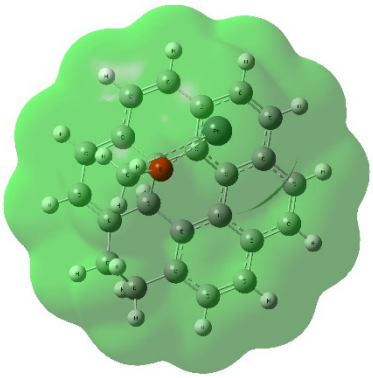
Graphite + NH_2 + Cr



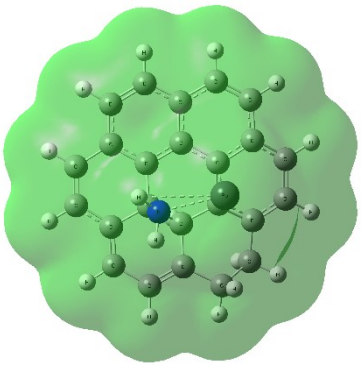
Graphite + OH + Pb



Graphite + COOH + Pb

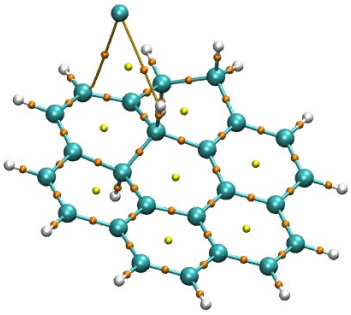


Graphite + OCH_3 + Pb

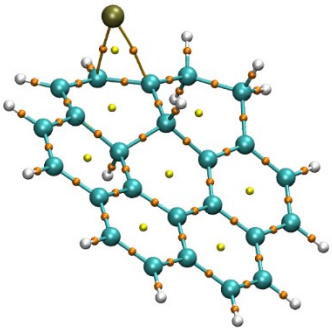


Graphite + NH_2 + Pb

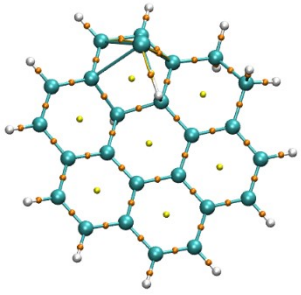
Figure S8 – MEPs showing interaction of metals with Graphite-like surfaces.



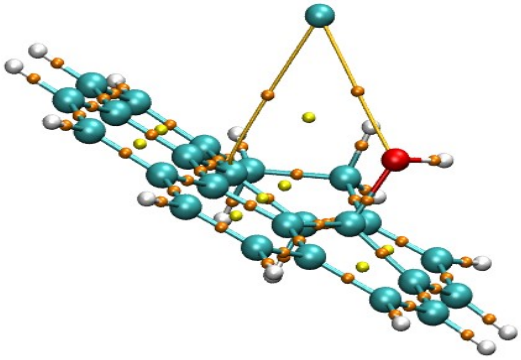
Graphite + Cd



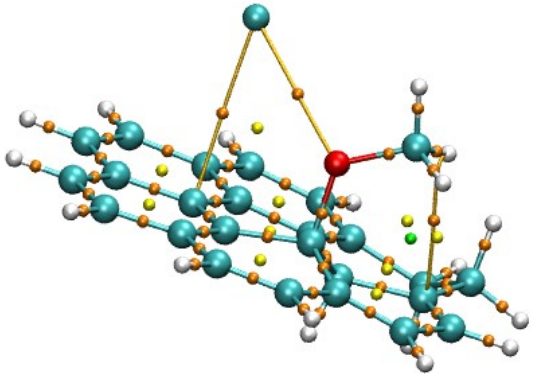
Graphite + Pb



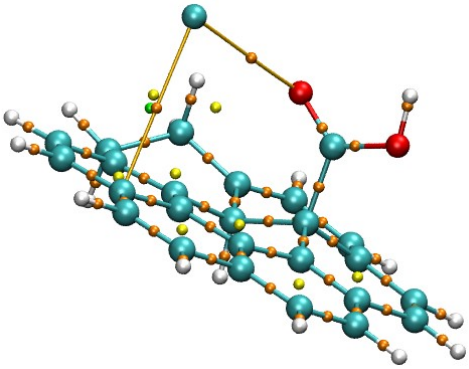
Graphite + Pb



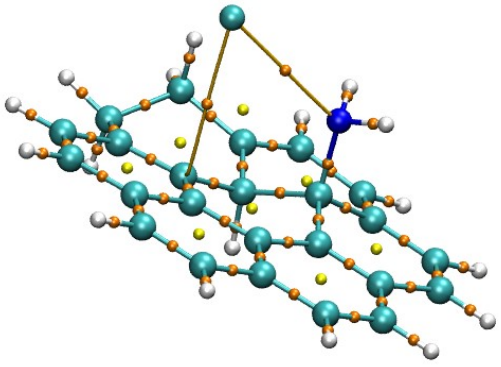
Graphite+ OH + Cd



Graphite+ OCH_3 + Cd

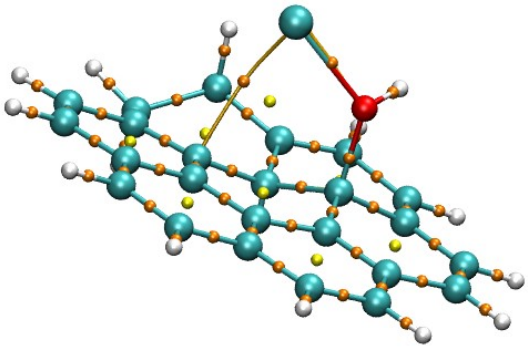


Graphite + COOH + Cd

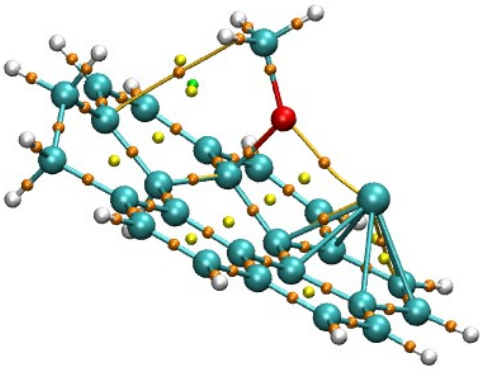


Graphite + NH_2+ Cd

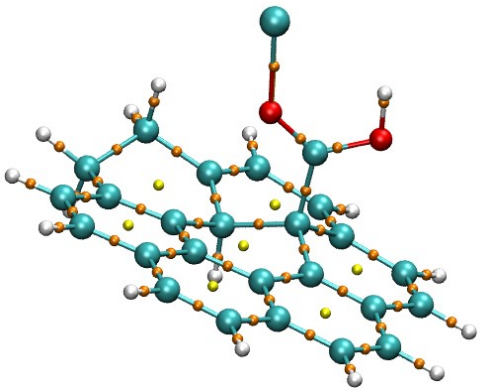
S9 – Bond critical points of all selected complexes



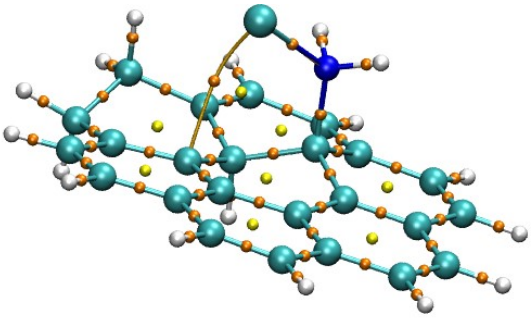
Graphite + OH + Cr



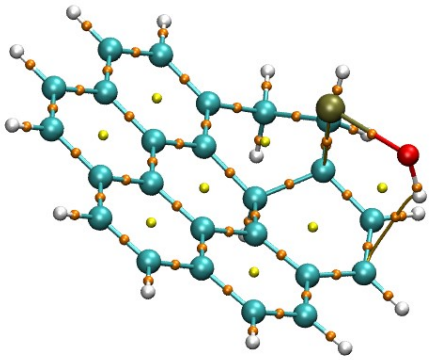
Graphite + OCH_3 + Cr



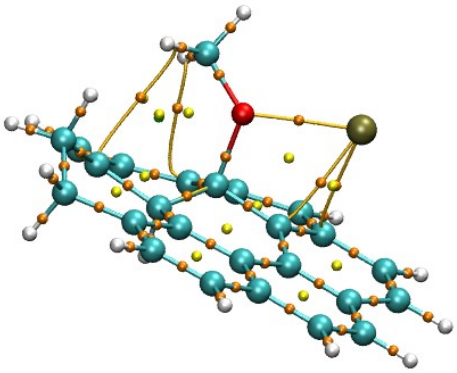
Graphite + COOH + Cr



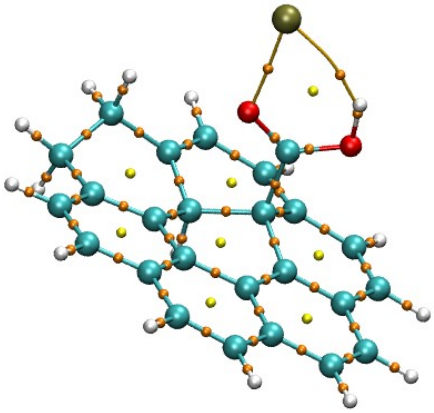
Graphite + NH_2 + Cr



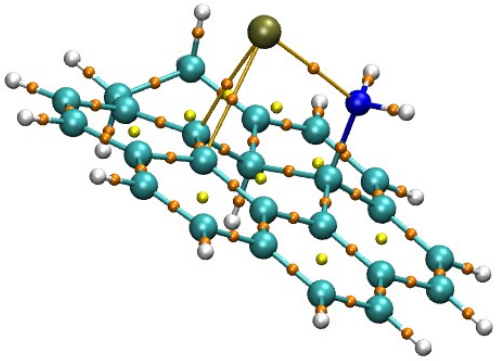
Graphite + OH + Pb



Graphite + OCH_3 + Pb



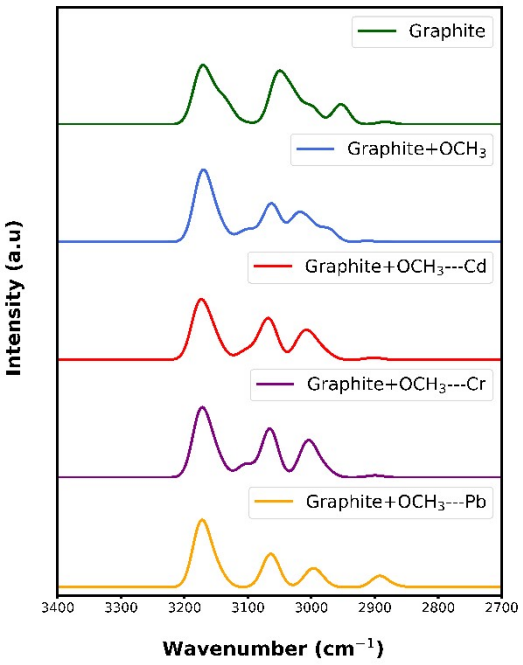
Graphite + COOH + Pb

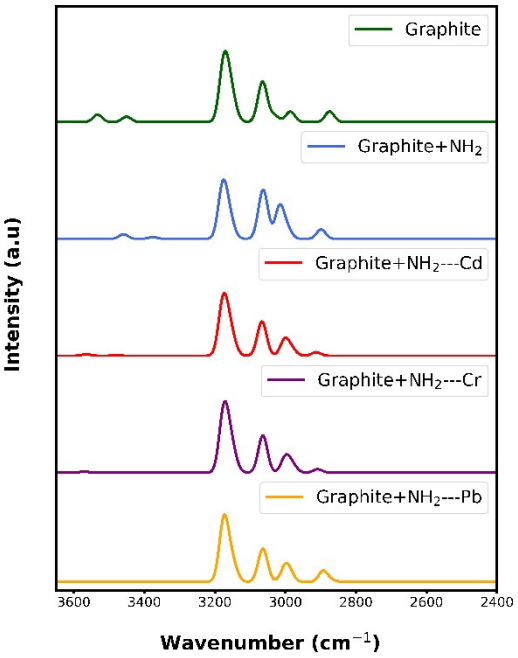


Graphite + NH_2 + Pb

Figure S2 – Images showing Bond Critical Points of complexes

S10 – Computer derived FT-IR spectra of all selected complexes


Graphite
Graphite+OCH3
Graphite+OCH3---Cd
Graphite+OCH3---Cr
Graphite+OCH3---Pb
Intensity (a.u)
3400 3300 3200 3100 3000 2900 2800 2700
Wavenumber (cm−1)


Graphite
Graphite+NH2
Graphite+NH2---Cd
Graphite+NH2---Cr
Graphite+NH2---Pb
Intensity (a.u)
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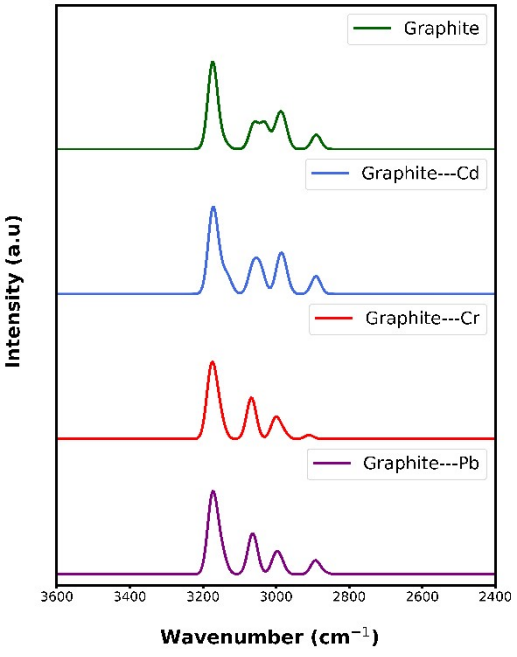
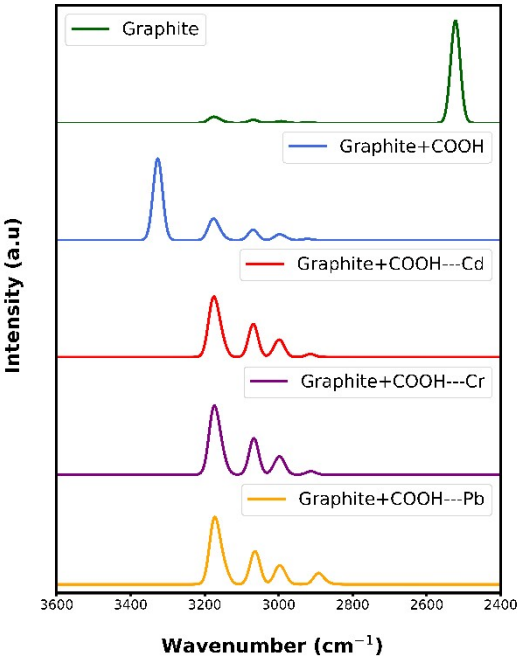
Wavenumber (cm−1)


Graphite
Graphite---Cd
Graphite---Cr
Graphite---Pb
Intensity (a.u)
3600 3400 3200 3000 2800 2600 2400
Wavenumber (cm−1)


Graphite
Graphite+COOH
Graphite+COOH---Cd
Graphite+COOH---Cr
Graphite+COOH---Pb
Intensity (a.u)
3600 3400 3200 3000 2800 2600 2400
Wavenumber (cm−1)

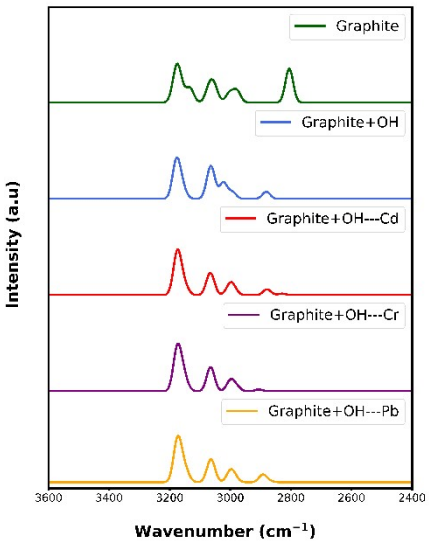


Figure S10 – Computationally derived FT-IR spectra of selected structures and their complexes with metals