Supplementary Information for

Exploration of spatial confinement and ligand effects for oxygen reduction reaction on Fe-N_x embedded hole-graphene

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1. Computational details of the adsorption free energies

In the four-electron reduction pathway of ORR, the intermediates include *O_2, *OOH, *OH, and *O. The adsorption free energies (ΔG_{ads}) of these intermediates were calculated relative to H_2O and H_2 under conditions of T = 298.15 K and pH = 0 (vs. SHE) according to equations[1, 2]:

$*+2H_2O \rightarrow *O_2 + 2H_2$:

$$\Delta G_{*O_2} = G_{*O_2} + 2G_{H_2} - G_* - 2G_{H_2O} \quad (1)$$

$*+2H_2O \rightarrow *OOH + 3/2H_2$:

$$\Delta G_{*OOH} = G_{*OOH} + 3/2G_{H_2} - G_* - 2G_{H_2O} \quad (2)$$

$*+H_2O \rightarrow *O + H_2$:

$$\Delta G_{*O} = G_{*O} + G_{H_2} - G_* - G_{H_2O} \quad (3)$$

$*+H_2O \rightarrow *OH + 1/2H_2$:

$$\Delta G_{*OH} = G_{*OH} + 1/2G_{H_2} - G_* - G_{H_2O} \quad (4)$$

where * represents the Fe-TCPP and Fe-$(mIM)_n$ (n=2-3) adsorption sites. The G of each intermediate is calculated from the total DFT ground state energy (E_{total}) corrected by the thermodynamic correction according to equation:

$$G = E_{total} + E_{ZPE} + \Delta H_{0\rightarrow T} - TS \quad (5)$$

where E_{ZPE} is zero-point energy calculated from the DFT frequency analysis. $\Delta H_{0\rightarrow T}$ is defined as the enthalpy variation by temperature and calculated as $\int_{0K}^{298K} C_P dT$ (C_p represents the heat capacities). S is the entropy at 298.15 K.

2. Computational details of the reaction free energy.

The reaction free energy (ΔG) of each ORR elemental step was calculated according to equation:

$$\Delta G = \Delta\Delta G_{ads} + \Delta G_{pH} + \Delta G_U \quad (6)$$

where ΔG of each ORR elemental step was calculated based on the computational hydrogen electrode (CHE) model developed by Nørskov et al[3]. $\Delta\Delta G_{ads}$ is the adsorption free energy variation between the reactants and products according to equations (1)-(4). $\Delta G_{pH} = -kT\ln[H^+] = pH\cdot kT\cdot\ln 10$ is used to correct the free energy of $H^+ + e^-$ referenced by a standard hydrogen electrode (SHE) at various pH values. $\Delta G_U = -neU$ is the free energy change resulting from an extra applied potential U *vs.* SHE.

The theoretical ORR overpotentials (η_{ORR}, *vs.* SHE) associated with different active sites were calculated according to equation

$$\eta_{ORR} = 1.23\ V + \Delta G_{max} \quad (7)$$

where 1.23 V is defined as the equilibrium potential of the overall 4-electron ORR at the standard state and ΔG_{max} represents the most positive free energy variation associated with the proton-electron-transfer (PET) steps.

3. Construction of the model of Fe-N_x embedded hole-graphene

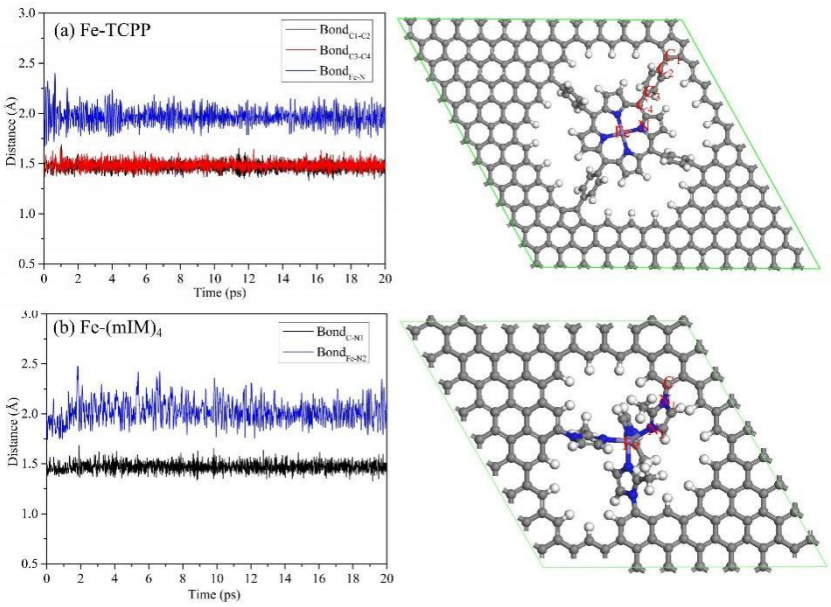

Fig. S1. The time evolution of the distances of the C-C bond, N-C bond, and Fe-C bond on Fe-TCPP and Fe-(mIM)$_4$ structures.

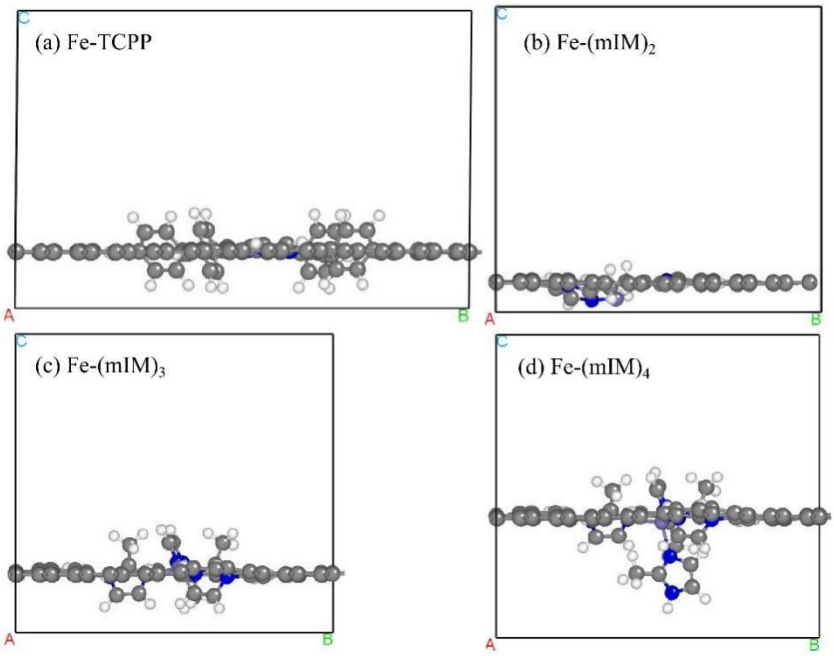

Fig. S2. Side views of the theoretical models of (a) Fe-TCPP, (b) Fe-(mIM)$_2$, (c) Fe-(mIM)$_3$, and (d) Fe-(mIM)$_4$. The gray, white, blue, and light blue spheres represent C, H, N, and Fe atoms, respectively. To avoid interactions between the models and their periodic images, a vacuum space (>15Å) was applied along the C-direction in the simulated cells.

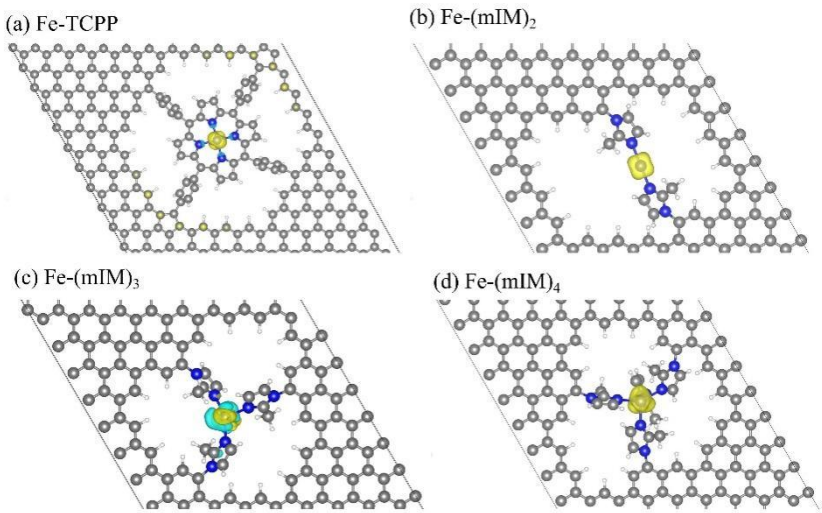

Fig. S3. The Spin density of (a) Fe-TCPP, (b) Fe-(mIM)$_2$, (c) Fe-(mIM)$_3$ and (d) Fe-(mIM)$_4$ embedded hole-graphene, respectively. Yellow and light blue surfaces are spin-up and spin-down density, respectively.

4. ORR reaction pathways and free-energy diagrams

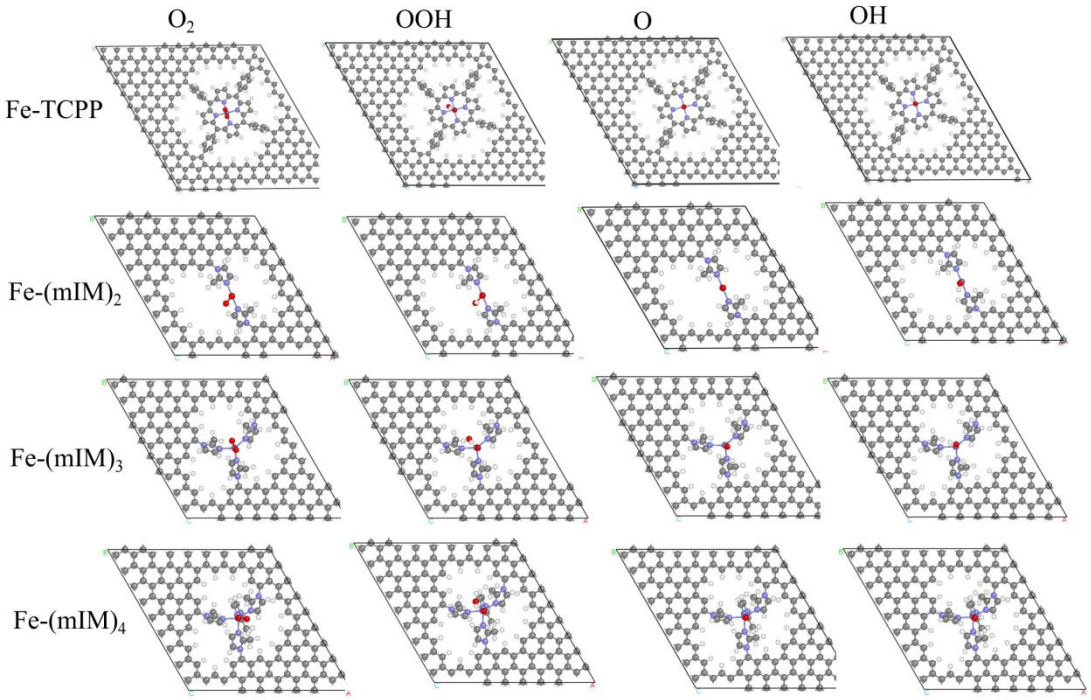

Fig. S4. The most stable adsorption structures of the key intermediates (*O_2, *OOH, *OH, and *O) on Fe-TCPP, (c) Fe-(mIM)$_2$, (d) Fe-(mIM)$_3$ and (e) Fe-(mIM)$_4$, respectively. The gray, white, blue, light blue and red spheres represent C, H, N, Fe, and O atoms, respectively.

5. Exploring the impact of spatial confinement on ORR

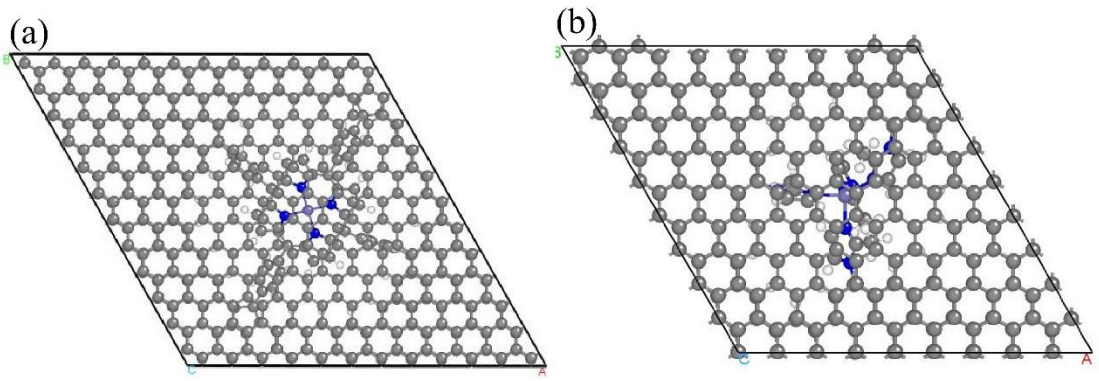

Fig. S5. Top view of the structure models used to simulate axial confinement. (a) Fe-TCPP and (b) Fe-$(mIM)_4$ active sites are on the underlying graphene layer, respectively. The gray, white, blue, and light blue spheres represent C, H, N, and Fe atoms, respectively.

6. Exploring the impact of axial ligand on ORR

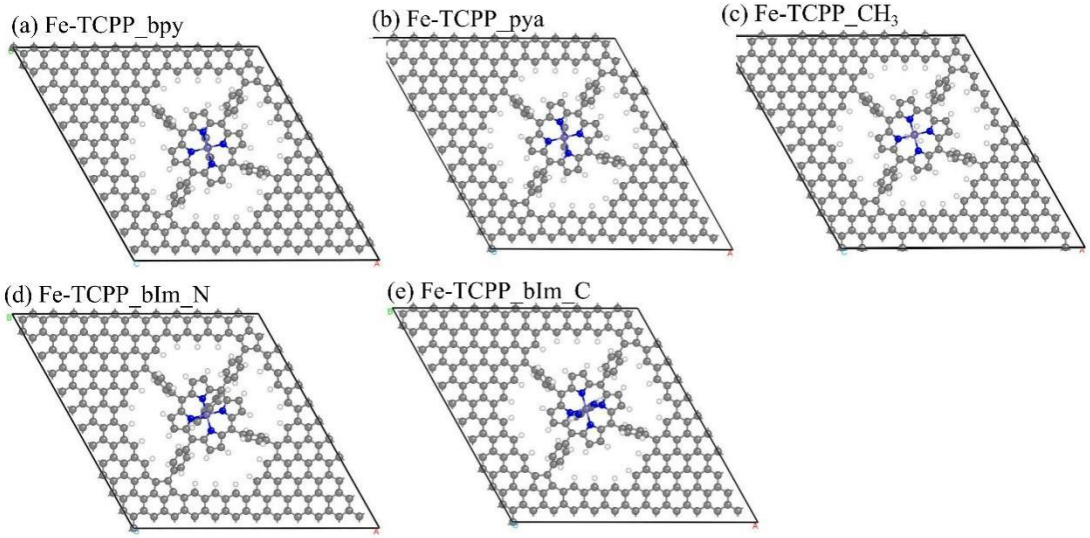

Fig. S6. Top view of the structure models of axial ligand decorated Fe-PCPP. The gray, white, blue, and light blue spheres represent C, H, N, and Fe atoms, respectively.

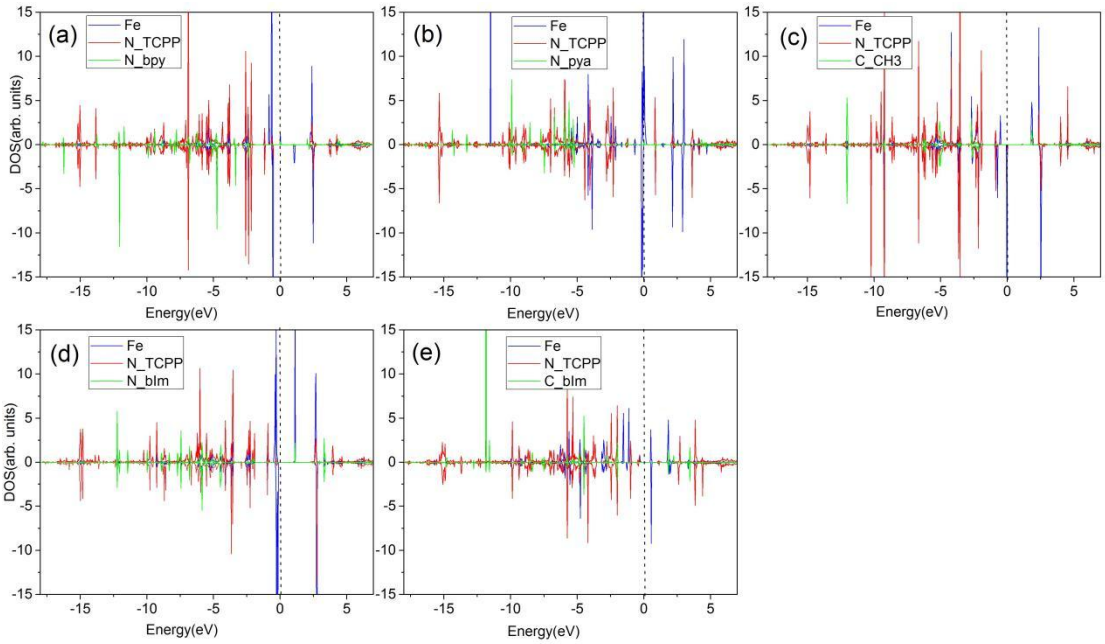

Fig. S7. The DOS of (a) Fe-TCPP_bpy, (b) Fe-TCPP_pya, (c) Fe-TCPP_CH_3, (d) Fe-TCPP_bIm_N and (e) Fe-TCPP_bIm_C structures. The dashed line indicates the Fermi energy level. The DOS of Fe (active site center) and the nearby N or C atoms are given in the figure.

7. The scaling relation and volcano plot

Table S1 Adsorption free energies (eV) of the key ORR intermediates (*OOH, *O, and *OH) and overpotential (η_{ORR}) on active sites.

Structures	ΔG_{*OH}	ΔG_{*O}	ΔG_{*OOH}	η_{ORR}
Fe-TCPP	0.94	1.56	4.01	0.61
Fe-$(mIM)_4$	0.52	0.85	3.59	0.89
Fe-TCPP_5Å	0.95	1.39	3.97	0.79
Fe-TCPP_6Å	0.61	1.28	3.71	0.62
Fe-TCPP_7Å	0.77	1.40	3.92	0.59
Fe-TCPP_8Å	0.73	1.66	3.93	0.50
Fe-TCPP_9Å	0.92	1.59	4.03	0.56
Fe-TCPP_10Å	0.84	1.49	3.93	0.59
Fe-TCPP_11Å	0.85	1.49	3.87	0.59
Fe-TCPP_12Å	0.80	1.43	3.78	0.60
Fe-TCPP_13Å	0.63	1.26	3.64	0.60
Fe-TCPP_14Å	0.86	1.47	3.91	0.62
Fe-$(mIM)_4$_5Å	1.04	1.32	4.25	0.96
Fe-$(mIM)_4$_6Å	0.78	1.16	4.08	0.85
Fe-$(mIM)_4$_7Å	0.65	1.08	3.91	0.80
Fe-$(mIM)_4$_8Å	0.67	1.21	3.88	0.69
Fe-$(mIM)_4$_9Å	0.59	1.49	3.72	0.64
Fe-$(mIM)_4$_10Å	0.60	0.91	3.67	0.92

Fe-$(mIM)_4$_11Å	0.63	1.01	3.68	0.85
Fe-$(mIM)_4$_12Å	0.55	0.91	3.58	0.87
Fe-$(mIM)_4$_13Å	0.54	0.92	3.60	0.86
Fe-$(mIM)_4$_14Å	0.65	1.01	3.71	0.87
Fe-TCPP_bpy	0.79	1.79	3.88	0.44
Fe-TCPP_pya	0.81	1.82	3.92	0.42
Fe-TCPP_CH_3	1.24	2.74	4.49	0.80
Fe-TCPP_bIm_C	0.95	1.55	3.69	0.62
Fe-TCPP_bIm_N	1.14	2.31	4.14	0.45

8. Coordinates of the Fe-TCPP and Fe-$(mIM)_4$ embeded hole-graphene.

Table S2 Fe-TCPP embeded hole-graphene

Lattice parameters	a = b = 29.52, c=18.0; α=β=90˚,γ=120˚				
atom	*x, y, z*	atom	*x, y, z*	atom	*x, y, z*
C	0.00462, 0.00235, 0.17714	C	0.02877, 0.47168, 0.17728	C	0.92466, 0.92193, 0.18042
C	0.03101, 0.05680, 0.17632	C	0.08456, 0.41541, 0.17711	C	0.94994, 0.97540, 0.17866
C	0.08691, 0.00124, 0.17760	C	0.11224, 0.47097, 0.17748	C	0.67653, 0.64442, 0.18445
C	0.11345, 0.05576, 0.17716	C	0.16779, 0.41422, 0.17893	C	0.63128, 0.64724, 0.17671
C	0.16966, 0.00081, 0.17797	C	0.19394, 0.46915, 0.17923	C	0.80602, 0.75347, 0.12258
C	0.19731, 0.05624, 0.17833	C	0.83293, 0.41558, 0.18239	C	0.72551, 0.59671, 0.20039
C	0.25229, 0.00121, 0.17721	C	0.86180, 0.47095, 0.18378	C	0.81848, 0.78731, 0.18286
C	0.27976, 0.05731, 0.17755	C	0.91714, 0.41604, 0.17951	C	0.86675, 0.83630, 0.18133
C	0.33502, 0.99981, 0.17674	C	0.94498, 0.47191, 0.17966	C	0.78483, 0.77392, 0.24455
C	0.36237, 0.05536, 0.17666	C	0.00045, 0.49952, 0.17832	C	0.67822, 0.59851, 0.19041
C	0.41830, 0.99884, 0.17667	C	0.02858, 0.55563, 0.17843	C	0.73874, 0.72692, 0.24552
C	0.44578, 0.05448, 0.17644	C	0.08439, 0.49900, 0.17722	C	0.72605, 0.69353, 0.18478
C	0.50192, 0.99844, 0.17636	C	0.11242, 0.55502, 0.17692	C	0.75975, 0.70673, 0.12334
C	0.52930, 0.05406, 0.17639	C	0.16827, 0.49788, 0.17860	C	0.63091, 0.69543, 0.16771
C	0.58582, 0.99804, 0.17551	C	0.19673, 0.55491, 0.17897	C	0.44729, 0.41714, 0.18138
C	0.61324, 0.05367, 0.17584	C	0.91591, 0.49948, 0.18160	C	0.49338, 0.41449, 0.17849
C	0.66978, 0.99835, 0.17547	C	0.94466, 0.55686, 0.18139	C	0.31668, 0.30792, 0.11926
C	0.69713, 0.05401, 0.17590	C	0.00085, 0.58384, 0.17969	C	0.39840, 0.46636, 0.19156
C	0.75384, 0.99876, 0.17640	C	0.02905, 0.63963, 0.17930	C	0.30204, 0.27210, 0.17857
C	0.78087, 0.05429, 0.17631	C	0.08422, 0.58289, 0.17701	C	0.25275, 0.22265, 0.17761
C	0.83718, 0.99844, 0.17788	C	0.11231, 0.63875, 0.17658	C	0.33586, 0.28501, 0.23905
C	0.86421, 0.05448, 0.17714	C	0.16777, 0.58250, 0.17713	C	0.44569, 0.46378, 0.18432
C	0.92032, 0.00111, 0.17835	C	0.19562, 0.63824, 0.17640	C	0.38240, 0.33201, 0.24048
C	0.94757, 0.05643, 0.17693	C	0.25055, 0.58306, 0.18108	C	0.39713, 0.36743, 0.18088
C	0.00286, 0.08439, 0.17621	C	0.27891, 0.63817, 0.18018	C	0.36355, 0.35457, 0.12026
C	0.03053, 0.13954, 0.17581	C	0.91961, 0.58634, 0.18216	C	0.49505, 0.36662, 0.17323
C	0.08552, 0.08343, 0.17629	C	0.94637, 0.64156, 0.18133	C	0.49564, 0.60106, 0.18027
C	0.11248, 0.13819, 0.17587	C	0.00215, 0.66850, 0.18007	C	0.54969, 0.62782, 0.17475
C	0.16825, 0.08264, 0.17773	C	0.02966, 0.72389, 0.17881	C	0.43887, 0.68467, 0.11355
C	0.19380, 0.13637, 0.17769	C	0.08472, 0.66698, 0.17765	C	0.41187, 0.51769, 0.19187
C	0.25220, 0.08620, 0.17825	C	0.11264, 0.72257, 0.17712	C	0.44269, 0.71402, 0.17700
C	0.27965, 0.14406, 0.17839	C	0.16776, 0.66632, 0.17580	C	0.46178, 0.70363, 0.24222
C	0.33480, 0.08382, 0.17684	C	0.19585, 0.72189, 0.17586	C	0.46740, 0.54692, 0.18463
C	0.36215, 0.13991, 0.17660	C	0.25084, 0.66614, 0.17745	C	0.47597, 0.66497, 0.24414

C	0.41756, 0.08217, 0.17628	C	0.27919, 0.72158, 0.17675	C	0.47168, 0.63543, 0.18086
C	0.44484, 0.13794, 0.17598	C	0.33333, 0.66549, 0.18133	C	0.45307, 0.64600, 0.11542
C	0.50135, 0.08203, 0.17646	C	0.36254, 0.72035, 0.17828	C	0.58015, 0.68343, 0.16677
C	0.52840, 0.13809, 0.17612	C	0.91977, 0.67028, 0.18161	C	0.62998, 0.46265, 0.18098
C	0.58533, 0.08188, 0.17607	C	0.94593, 0.72504, 0.18040	C	0.57594, 0.43487, 0.17741
C	0.61286, 0.13722, 0.17639	C	0.00194, 0.75208, 0.17874	C	0.73256, 0.42893, 0.11774
C	0.66900, 0.08164, 0.17619	C	0.02916, 0.80725, 0.17755	C	0.71253, 0.54569, 0.19821
C	0.69656, 0.13711, 0.17667	C	0.08517, 0.75099, 0.17748	C	0.74370, 0.41133, 0.18388
C	0.75261, 0.08189, 0.17637	C	0.11296, 0.80633, 0.17662	C	0.71430, 0.40740, 0.24796
C	0.78008, 0.13741, 0.17681	C	0.16816, 0.75002, 0.17613	C	0.65720, 0.51649, 0.18782
C	0.83614, 0.08214, 0.17662	C	0.19612, 0.80558, 0.17599	C	0.67492, 0.42052, 0.24593
C	0.86357, 0.13778, 0.17644	C	0.25137, 0.74962, 0.17598	C	0.66407, 0.43845, 0.17991
C	0.91942, 0.08355, 0.17667	C	0.27935, 0.80509, 0.17605	C	0.69334, 0.44231, 0.11586
C	0.94705, 0.13894, 0.17610	C	0.33469, 0.74896, 0.17712	C	0.54615, 0.37931, 0.17254
C	0.00254, 0.16697, 0.17599	C	0.36267, 0.80428, 0.17664	H	0.83261, 0.76499, 0.07491
C	0.03107, 0.22206, 0.17608	C	0.41808, 0.74766, 0.17746	H	0.76350, 0.63042, 0.20814
C	0.08602, 0.16708, 0.17563	C	0.44604, 0.80277, 0.17728	H	0.79575, 0.80031, 0.29159
C	0.11623, 0.22197, 0.17606	C	0.91878, 0.75391, 0.18052	H	0.71226, 0.71542, 0.29326
C	0.16625, 0.16383, 0.17599	C	0.94350, 0.80826, 0.17905	H	0.74888, 0.68045, 0.07618
C	0.20068, 0.21791, 0.17565	C	0.00107, 0.83538, 0.17782	H	0.66526, 0.73339, 0.16258
C	0.24795, 0.17066, 0.17905	C	0.03145, 0.89037, 0.17752	H	0.29131, 0.29831, 0.07139
C	0.33392, 0.16788, 0.17752	C	0.08517, 0.83445, 0.17667	H	0.35984, 0.43277, 0.19665
C	0.41683, 0.16529, 0.17575	C	0.11395, 0.88975, 0.17678	H	0.32477, 0.25802, 0.28600
C	0.49981, 0.16403, 0.17572	C	0.16857, 0.83376, 0.17628	H	0.40768, 0.34165, 0.28848
C	0.58538, 0.16625, 0.17617	C	0.19677, 0.88919, 0.17633	H	0.37485, 0.38141, 0.07310
C	0.61347, 0.22009, 0.17612	C	0.25167, 0.83323, 0.17607	H	0.46112, 0.32829, 0.17013
C	0.66851, 0.16500, 0.17679	C	0.27965, 0.88875, 0.17647	H	0.42357, 0.69174, 0.06256
C	0.69639, 0.22021, 0.17755	C	0.33487, 0.83248, 0.17630	H	0.38670, 0.53475, 0.19650
C	0.75205, 0.16516, 0.17701	C	0.36293, 0.88797, 0.17658	H	0.46443, 0.72540, 0.29249
C	0.77976, 0.22073, 0.17752	C	0.41824, 0.83153, 0.17705	H	0.49134, 0.65789, 0.29508
C	0.83553, 0.16543, 0.17667	C	0.44641, 0.88695, 0.17663	H	0.45054, 0.62427, 0.06521
C	0.86317, 0.22105, 0.17708	C	0.50134, 0.83151, 0.17633	H	0.56445, 0.70958, 0.16086
C	0.91901, 0.16627, 0.17628	C	0.52970, 0.88552, 0.17611	H	0.75420, 0.43112, 0.06705
C	0.94681, 0.22158, 0.17654	C	0.61637, 0.88884, 0.17623	H	0.73791, 0.52907, 0.20366
C	0.00252, 0.24938, 0.17646	C	0.70023, 0.88880, 0.17806	H	0.72192, 0.39293, 0.29951
C	0.02968, 0.30461, 0.17667	C	0.78404, 0.88800, 0.18005	H	0.65318, 0.41824, 0.29655
C	0.08726, 0.24941, 0.17646	C	0.87068, 0.88749, 0.18231	H	0.68582, 0.45701, 0.06446
C	0.11375, 0.30436, 0.17743	C	0.91804, 0.84059, 0.17879	H	0.56281, 0.35374, 0.16930
C	0.17409, 0.24950, 0.17637	C	0.95226, 0.89459, 0.17874	H	0.67324, 0.32293, 0.17757
C	0.19790, 0.30373, 0.17781	C	0.00573, 0.91992, 0.17790	H	0.59359, 0.24291, 0.17569
C	0.66848, 0.24834, 0.17726	C	0.03251, 0.97466, 0.17755	H	0.51958, 0.20641, 0.17499
C	0.69573, 0.30274, 0.17842	C	0.08671, 0.91787, 0.17726	H	0.43860, 0.20780, 0.17528
C	0.75176, 0.24851, 0.17821	C	0.11454, 0.97315, 0.17783	H	0.35668, 0.21029, 0.17752
C	0.77913, 0.30395, 0.17961	C	0.16932, 0.91733, 0.17674	H	0.83925, 0.49112, 0.18609
C	0.83515, 0.24885, 0.17780	C	0.19711, 0.97284, 0.17745	H	0.87725, 0.56704, 0.18301
C	0.86259, 0.30445, 0.17881	C	0.25205, 0.91698, 0.17639	H	0.87726, 0.64917, 0.18245
C	0.91864, 0.24919, 0.17682	C	0.27978, 0.97272, 0.17673	H	0.87639, 0.73185, 0.18173
C	0.94612, 0.30474, 0.17720	C	0.33509, 0.91611, 0.17671	H	0.76209, 0.84557, 0.18118
C	0.00159, 0.33247, 0.17679	C	0.36280, 0.97161, 0.17668	H	0.67913, 0.84630, 0.17894
C	0.02895, 0.38795, 0.17686	C	0.41848, 0.91526, 0.17667	H	0.59694, 0.84644, 0.17655
C	0.08525, 0.33191, 0.17724	C	0.44617, 0.97075, 0.17669	H	0.52155, 0.80896, 0.17554
C	0.11213, 0.38712, 0.17765	C	0.50222, 0.91469, 0.17643	H	0.35350, 0.64304, 0.18440
C	0.16980, 0.33173, 0.17855	C	0.52976, 0.97008, 0.17605	H	0.27331, 0.56310, 0.18311
C	0.19526, 0.38640, 0.17960	C	0.58705, 0.91408, 0.17565	H	0.23630, 0.48886, 0.17998
C	0.75059, 0.33179, 0.18063	C	0.61401, 0.97031, 0.17552	H	0.23772, 0.40817, 0.18058
C	0.77784, 0.38730, 0.18294	C	0.67153, 0.91545, 0.17662	H	0.24028, 0.32653, 0.17857

C	0.83443, 0.33215, 0.17994	C	0.69850, 0.97127, 0.17605	Fe	0.56212, 0.53110, 0.18111
C	0.86172, 0.38778, 0.18051	C	0.75508, 0.91505, 0.17820	N	0.63598, 0.54917, 0.18485
C	0.91809, 0.33261, 0.17809	C	0.78206, 0.97109, 0.17726	N	0.48829, 0.51352, 0.18144
C	0.94547, 0.38822, 0.17823	C	0.83840, 0.91289, 0.18077	N	0.58143, 0.60549, 0.17889
C	0.00097, 0.41593, 0.17723	C	0.86540, 0.97049, 0.17923	N	0.54329, 0.45660, 0.18019

Table S3 Fe-$(mIM)_4$ embeded hole-graphene

Lattice parameters	a = b = 22.14, c=20.0; α=β=90°,γ=120°				
atom	*x, y, z*	atom	*x, y, z*	atom	*x, y, z*
C	0. 99519, 0. 99901, 0. 36013	C	0. 14718, 0. 63056, 0. 35969	C	0. 42649, 0. 30897, 0. 29921
C	0. 03263, 0. 07326, 0. 35958	C	0. 22168, 0. 55677, 0. 36632	C	0. 44378, 0. 49768, 0. 43988
C	0. 10591, 0. 99813, 0. 36248	C	0. 25841, 0. 63094, 0. 36454	C	0. 42638, 0. 53556, 0. 34512
C	0. 14356, 0. 07220, 0. 36432	C	0. 89042, 0. 55695, 0. 38104	C	0. 42561, 0. 55500, 0. 27397
C	0. 21752, 0. 99870, 0. 36395	C	0. 92571, 0. 63015, 0. 37950	C	0. 76432, 0. 62647, 0. 29903
C	0. 25376, 0. 07252, 0. 36899	C	0. 99904, 0. 66707, 0. 36825	C	0. 70441, 0. 56356, 0. 30357
C	0. 32973, 0. 00046, 0. 36232	C	0. 03427, 0. 74058, 0. 36397	C	0. 70025, 0. 62804, 0. 38431
C	0. 36640, 0. 07463, 0. 36579	C	0. 10999, 0. 66742, 0. 35997	C	0. 67928, 0. 65012, 0. 44624
C	0. 44154, 0. 00236, 0. 35839	C	0. 14611, 0. 74127, 0. 35879	C	0. 50874, 0. 35458, 0. 37786
C	0. 47846, 0. 07694, 0. 35852	C	0. 22104, 0. 66776, 0. 36037	C	0. 55374, 0. 36052, 0. 43566
C	0. 55307, 0. 00343, 0. 35499	C	0. 25753, 0. 74182, 0. 35918	C	0. 59632, 0. 60676, 0. 15117
C	0. 58981, 0. 07740, 0. 35398	C	0. 33230, 0. 66838, 0. 36792	C	0. 58266, 0. 60190, 0. 21832
C	0. 66404, 0. 00335, 0. 35350	C	0. 36926, 0. 74323, 0. 36360	C	0. 57718, 0. 50389, 0. 18996
C	0. 70112, 0. 07755, 0. 35348	C	0. 88934, 0. 66680, 0. 38427	C	0. 57282, 0. 43450, 0. 19143
C	0. 77482, 0. 00216, 0. 35365	C	0. 92119, 0. 73799, 0. 37105	H	0. 35049, 0. 49204, 0. 49075
C	0. 81199, 0. 07618, 0. 35367	C	0. 99585, 0. 77645, 0. 36441	H	0. 45818, 0. 61118, 0. 26414
C	0. 88463, 0. 99989, 0. 35622	C	0. 03229, 0. 85026, 0. 36142	H	0. 37195, 0. 54019, 0. 26039
C	0. 92182, 0. 07387, 0. 35587	C	0. 10843, 0. 77776, 0. 35973	H	0. 44350, 0. 52755, 0. 24107
C	0. 99594, 0. 11061, 0. 35752	C	0. 14459, 0. 85149, 0. 35927	H	0. 43590, 0. 41053, 0. 27443
C	0. 03307, 0. 18457, 0. 35736	C	0. 22022, 0. 77846, 0. 35787	H	0. 38734, 0. 26855, 0. 26778
C	0. 10705, 0. 11101, 0. 36109	C	0. 25663, 0. 85255, 0. 35795	H	0. 46843, 0. 47936, 0. 47507
C	0. 14249, 0. 18341, 0. 35927	C	0. 33155, 0. 77951, 0. 36008	H	0. 80826, 0. 64595, 0. 26526
C	0. 21559, 0. 10687, 0. 36947	C	0. 36814, 0. 85361, 0. 35846	H	0. 65157, 0. 67874, 0. 43619
C	0. 32864, 0. 11039, 0. 37035	C	0. 44172, 0. 78181, 0. 36208	H	0. 72525, 0. 68401, 0. 47672
C	0. 44069, 0. 11313, 0. 36258	C	0. 47854, 0. 85409, 0. 35815	H	0. 64408, 0. 60356, 0. 47543
C	0. 55255, 0. 11454, 0. 35488	C	0. 59086, 0. 85676, 0. 35308	H	0. 53018, 0. 31152, 0. 46395
C	0. 58898, 0. 18919, 0. 35267	C	0. 70003, 0. 85537, 0. 35365	H	0. 60620, 0. 37218, 0. 42019
C	0. 66420, 0. 11467, 0. 35328	C	0. 81006, 0. 85185, 0. 35631	H	0. 56002, 0. 40285, 0. 46871
C	0. 70149, 0. 18876, 0. 35264	C	0. 88230, 0. 77441, 0. 36403	H	0. 68823, 0. 51761, 0. 27298
C	0. 77525, 0. 11360, 0. 35348	C	0. 91977, 0. 84909, 0. 36160	H	0. 57763, 0. 28014, 0. 34926
C	0. 81266, 0. 18735, 0. 35361	C	0. 99466, 0. 88703, 0. 36210	H	0. 67817, 0. 33065, 0. 34973
C	0. 88585, 0. 11212, 0. 35440	C	0. 03159, 0. 96091, 0. 36142	H	0. 78605, 0. 43678, 0. 35471
C	0. 92333, 0. 18615, 0. 35482	C	0. 10656, 0. 88754, 0. 36046	H	0. 83429, 0. 52974, 0. 38934
C	0. 99752, 0. 22280, 0. 35659	C	0. 14340, 0. 96161, 0. 36204	H	0. 83446, 0. 63659, 0. 39678
C	0. 03567, 0. 29692, 0. 35804	C	0. 21889, 0. 88892, 0. 35892	H	0. 56415, 0. 80005, 0. 35264
C	0. 10741, 0. 22138, 0. 35820	C	0. 25554, 0. 96272, 0. 36162	H	0. 47064, 0. 75424, 0. 36351
C	0. 14415, 0. 29464, 0. 35921	C	0. 33061, 0. 89020, 0. 35815	H	0. 42386, 0. 65821, 0. 38346
C	0. 66516, 0. 22724, 0. 35122	C	0. 36728, 0. 96429, 0. 35940	H	0. 25020, 0. 41833, 0. 37382
C	0. 70384, 0. 29956, 0. 35047	C	0. 44205, 0. 89156, 0. 35793	H	0. 20092, 0. 32058, 0. 35975
C	0. 77569, 0. 22466, 0. 35332	C	0. 47874, 0. 96596, 0. 35694	H	0. 19926, 0. 21340, 0. 35953

C	0.81387, 0.29842, 0.35411	C	0.55382, 0.89186, 0.35479	H	0.24321, 0.16322, 0.37336
C	0.88681, 0.22357, 0.35433	C	0.59017, 0.96632, 0.35416	H	0.33796, 0.21232, 0.37378
C	0.92483, 0.29760, 0.35576	C	0.66377, 0.89214, 0.35304	H	0.66887, 0.79866, 0.35471
C	0.99888, 0.33414, 0.35762	C	0.70108, 0.96644, 0.35335	H	0.71854, 0.75040, 0.34507
C	0.03626, 0.40847, 0.35934	C	0.77231, 0.88940, 0.35460	H	0.60772, 0.64772, 0.11516
C	0.11039, 0.33305, 0.36030	C	0.81067, 0.96390, 0.35458	H	0.61432, 0.43452, 0.16130
C	0.14864, 0.40874, 0.36375	C	0.88391, 0.88776, 0.35925	H	0.52252, 0.39219, 0.17321
C	0.77711, 0.33601, 0.35293	C	0.92150, 0.96232, 0.35870	H	0.57854, 0.42157, 0.24310
C	0.81506, 0.40902, 0.35620	C	0.36570, 0.18348, 0.37059	H	0.58086, 0.63989, 0.25121
C	0.88788, 0.33487, 0.35611	C	0.47769, 0.18792, 0.35967	H	0.60004, 0.53105, 0.08771
C	0.92493, 0.40869, 0.35925	C	0.43689, 0.22141, 0.36283	N	0.37459, 0.52705, 0.38835
C	0.99924, 0.44527, 0.36010	C	0.55061, 0.22358, 0.35311	N	0.50361, 0.40720, 0.35073
C	0.03638, 0.51962, 0.36101	C	0.22115, 0.44595, 0.36998	N	0.46246, 0.29326, 0.34657
C	0.11078, 0.44525, 0.36171	C	0.25856, 0.51905, 0.37180	N	0.47031, 0.51928, 0.37584
C	0.14760, 0.51934, 0.36263	C	0.33254, 0.55905, 0.37863	N	0.76194, 0.66729, 0.35029
C	0.88703, 0.44521, 0.36173	C	0.36754, 0.63071, 0.37659	N	0.66348, 0.56493, 0.35572
C	0.92491, 0.52022, 0.36932	C	0.80829, 0.74110, 0.35776	N	0.59241, 0.54445, 0.13404
C	0.99923, 0.55643, 0.36428	C	0.77463, 0.77917, 0.35317	N	0.57023, 0.53791, 0.24205
C	0.03601, 0.63027, 0.36395	C	0.38497, 0.50251, 0.44843	Fe	0.55700, 0.51271, 0.34369
C	0.11025, 0.55640, 0.36050	C	0.45138, 0.37878, 0.30291		

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