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Amorphous graphene: Electronic Supplementary Information

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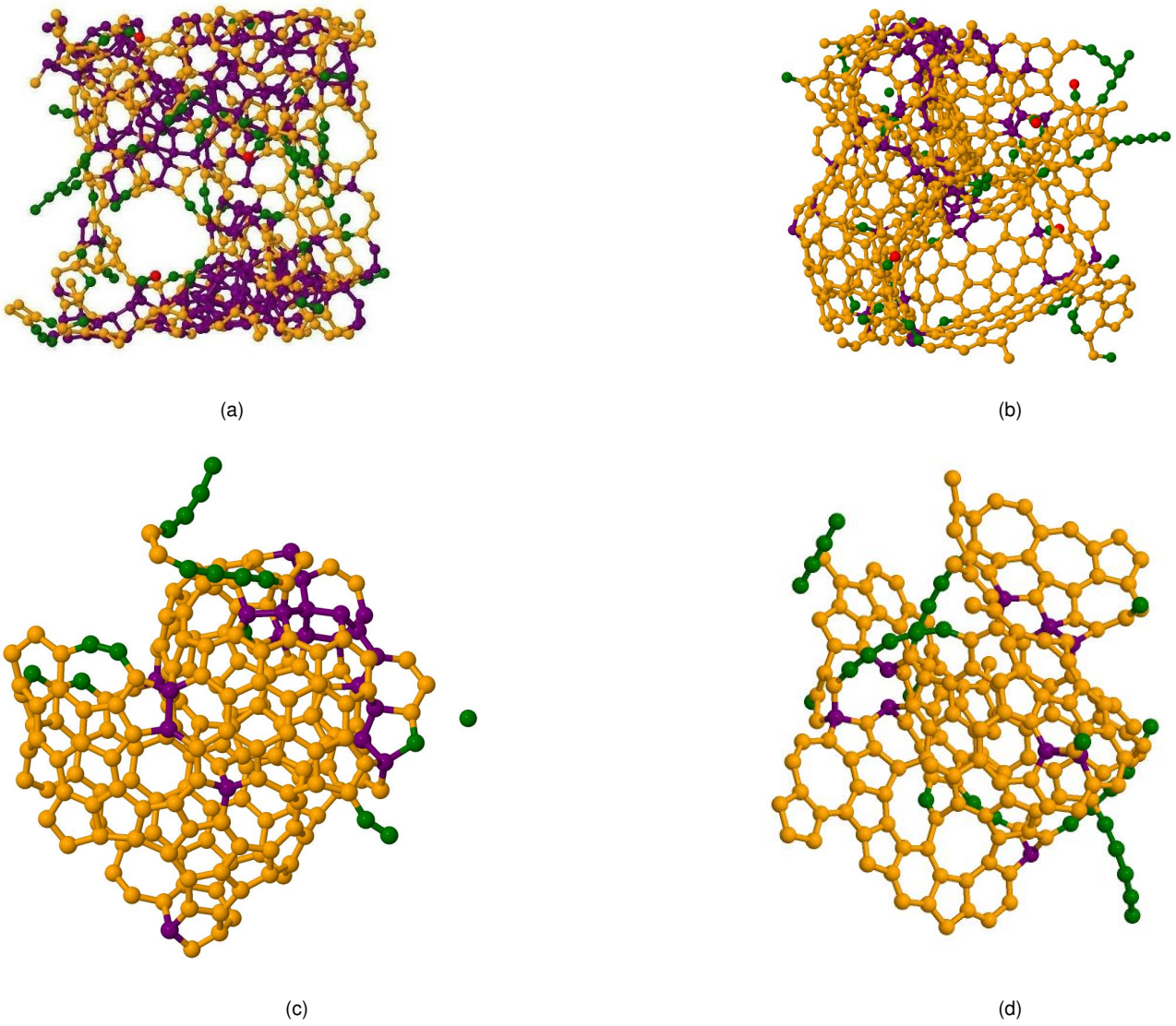

(a) (b) (c) (d)

Fig. 1 Structure models: (a) Melt-Quench (SIESTA, HARRIS) (648 atom), (b) FEAR (SIESTA, HARRIS) (648 atom) (c) FEAR (SIESTA, HARRIS) (216 atom), and (d) Melt-Quench (VASP, LDA). color coding: purple (sp^3), orange (sp^2), green (sp) and red (singly bonded).

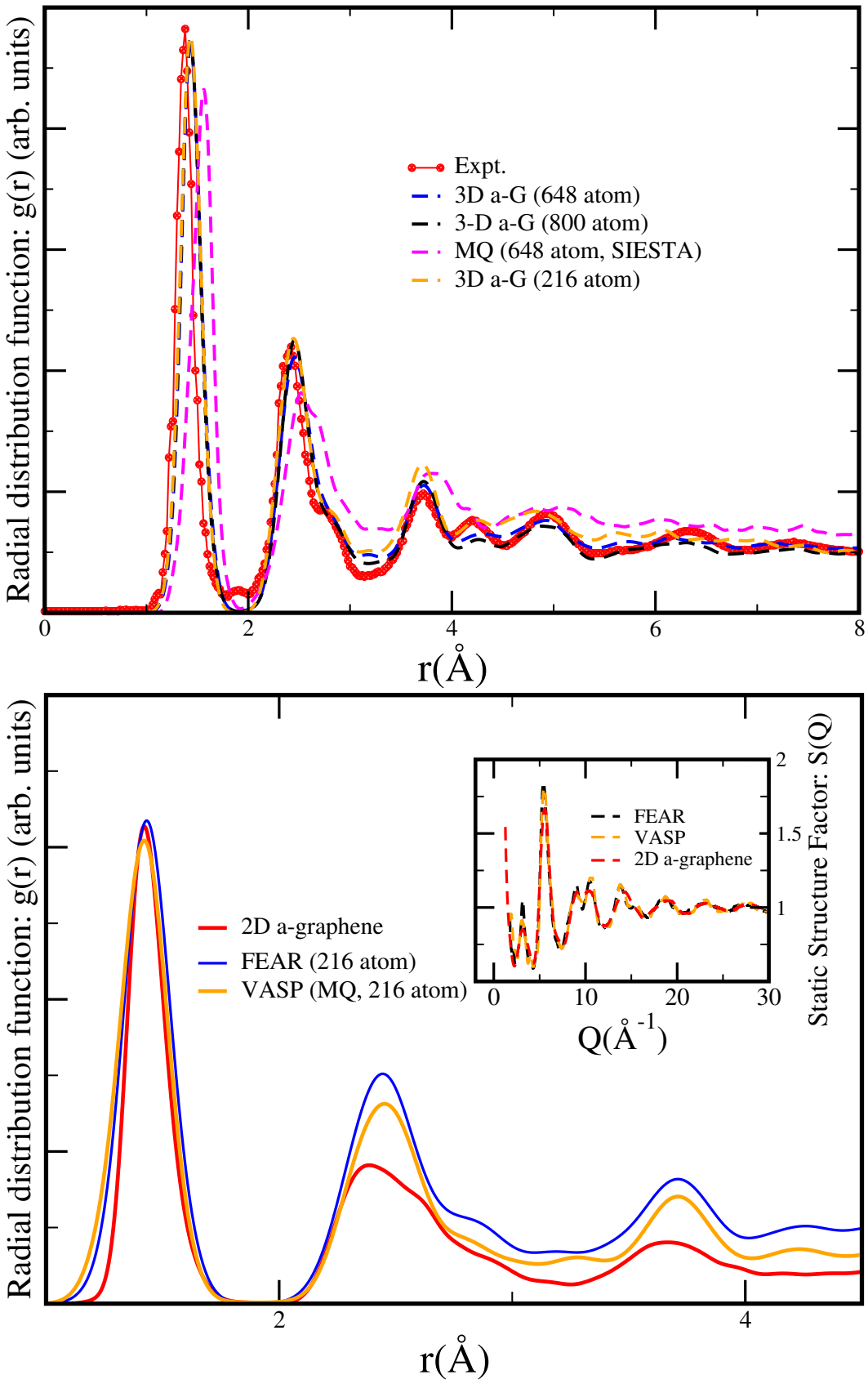

Fig. 2 (Top panel) Comparison of radial distribution function $g(r)$ for the 3 FEAR models, MQ (SIESTA, Harris) with the experimental data of nano-porous amorphous carbon (Ref.13, Farmahini et. al.) **(Bottom panel)** Comparison of radial distribution function $g(r)$ and $S(Q)$ (INSET) of 216-FEAR model, 216-VASP model and 800 atom 2D a-graphene model.

Table 1 Nomenclature and details of our models: Position of first (r_1) and second (r_2) peak of RDF, Mean co-ordination number (n), percentage of sp^3, sp^2 and sp, Free Energy per atom of the relaxed models (E_0) and the total simulation time (T_0).

Model	r_1(Å)	r_2(Å)	n	% of sp^3	% of sp^2	% of sp	$E_0(eV/atom)$ *	Total simulation time (T_0)†
FEAR-216	1.43	2.45	3.02	9.72	82.41	7.87	0.61	6.15
VASP-216	1.45	2.49	2.90	4.17	81.48	14.35	0.54	100.0
FEAR-648	1.43	2.46	3.00	10.80	79.00	9.57	0.67	–
SIESTA-648	1.57	2.53	3.28	41.05	45.68	12.65	–	45.12
FEAR-800	1.43	2.46	2.98	11.25	76.50	11.25	0.63	–
2D a-graphene	1.42	2.39	2.94	–	94.75	5.25	0.56	–
2D c-graphene	1.42	2.46	3.00	–	100.0	–	0.00	–
3D schwarzite	1.48	2.57	3.00	–	100.0	–	0.39	–

* *after substraction from lowest value of relaxed E_0 (2D c-graphene) obtained with VASP.*
† *Total CPU time for same number of cores.*

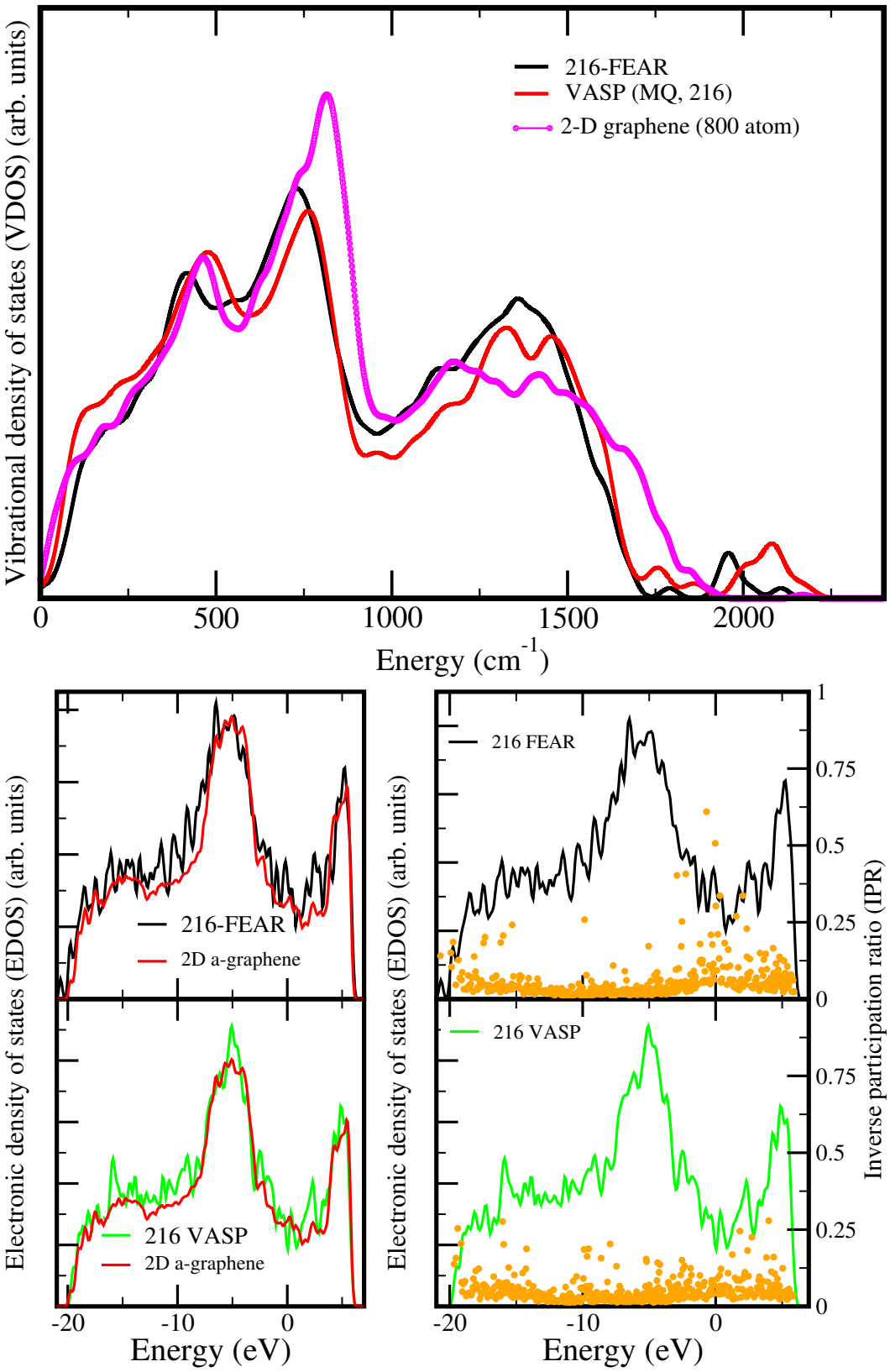

Fig. 3 (Top panel) Plot and comparison of vibrational density of states of 216 FEAR, 216 VASP (MQ) and 2D a-graphene (800 atoms). **(Bottom panel)** Plot and comparison of EDOS ($E_F = 0eV$) and localization (IPR, yellow dot) for the two model 216 FEAR and 216 VASP.