

# Monodispersed uranium atomic site on carbonaceous materials

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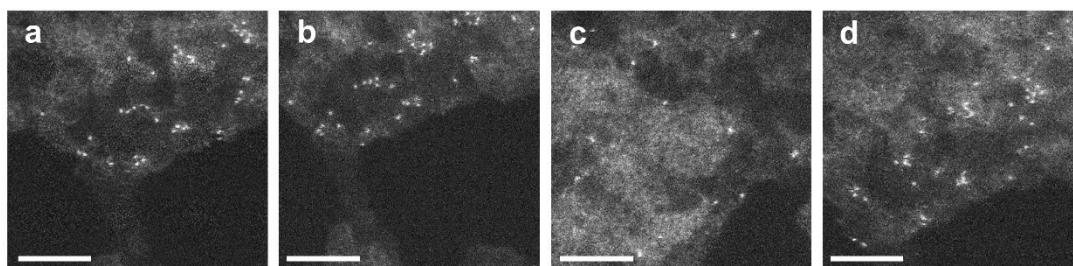


Figure. S1 STEM-HAADF images of four typical examples showing monodispersed uranium atomic site formed on amorphous carbon instead of graphene. Scale bar = 5

nm

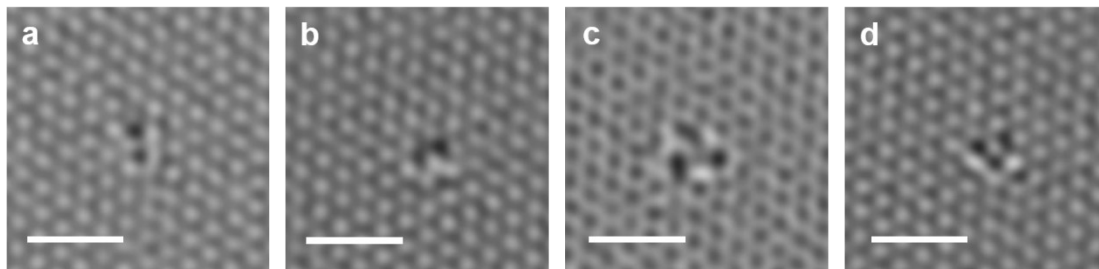


Figure. S2. Examples of uranium atom configuration on graphene in TEM mode after applying a mask. Scale bar = 1 nm

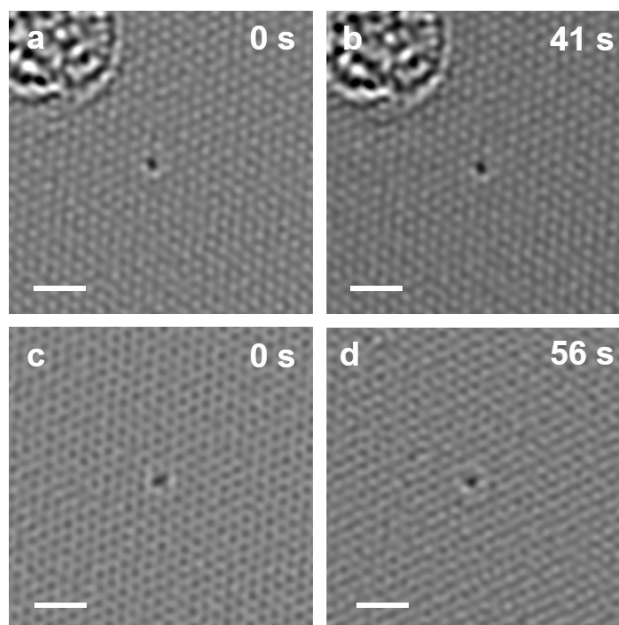


Figure. S3. Stability of single-atom uranium located at the hollow site and top site of carbon atom of perfect graphene. Scale bar = 1 nm

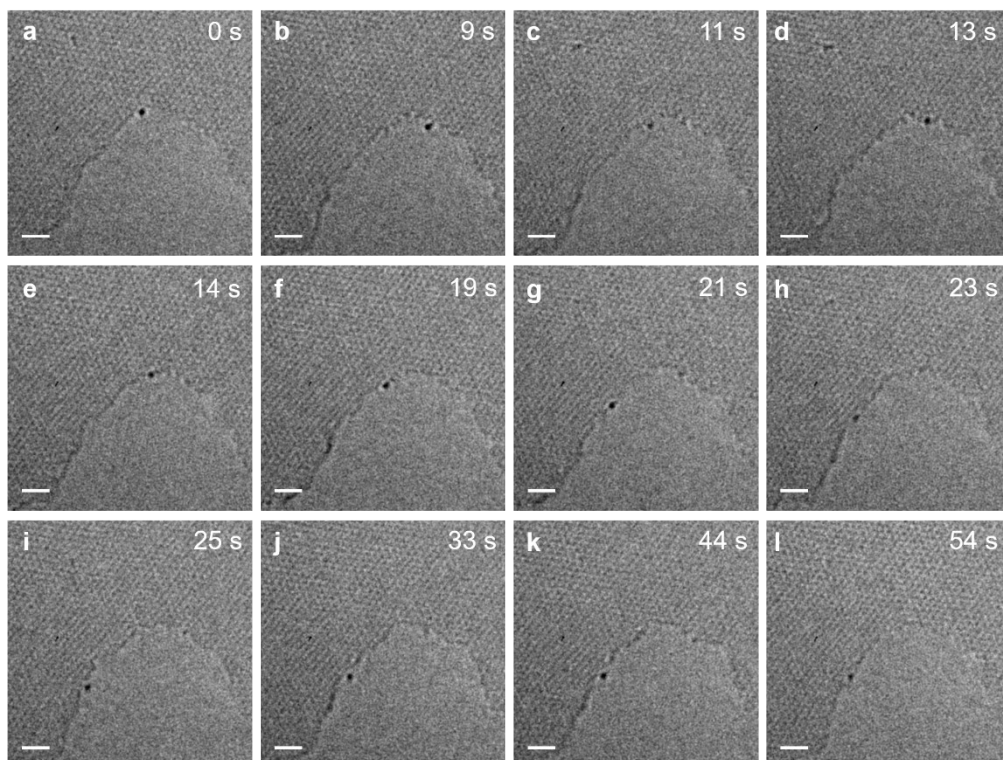


Figure. S4 Example of the movement of uranium atoms at the edge of graphene under electron beam irradiation. Scale bar = 1 nm

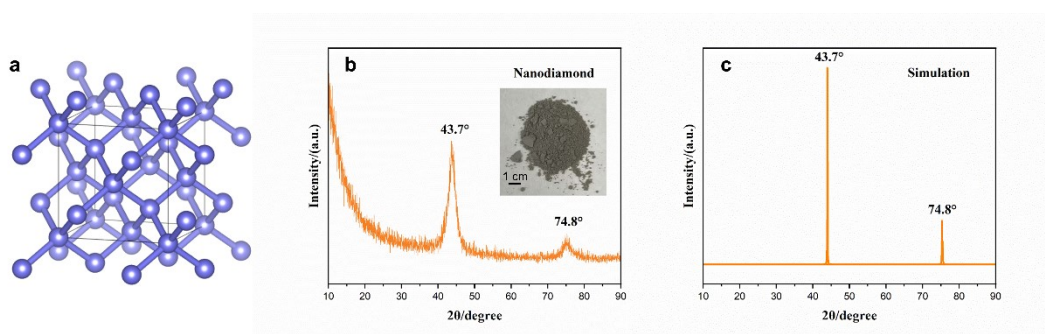


Figure S5: Lattice structure and XRD experimental and simulated spectra of nanodiamonds: (a) Lattice structure stick model; (b) XRD experimental diagram; (c) XRD simulation diagram.

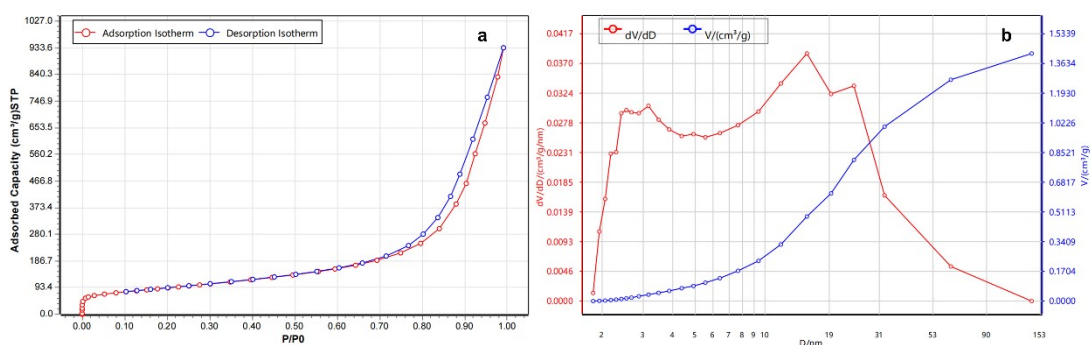


Figure S6: BET experiments of nanodiamonds: (a)  $N_2$  adsorption and desorption isotherm linear plot; (b) Pore volume and pore size curve measured by BJH adsorption method.

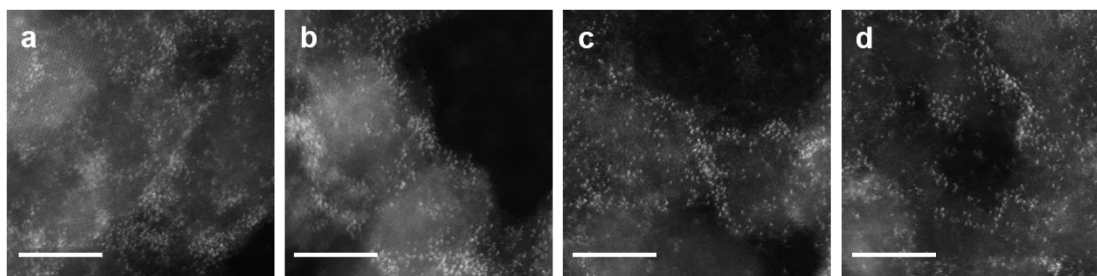


Figure. S7 Several examples of the distribution of uranyl ions adsorbed by nanodiamonds in STEM-HAADF mode. Scale bar = 5 nm

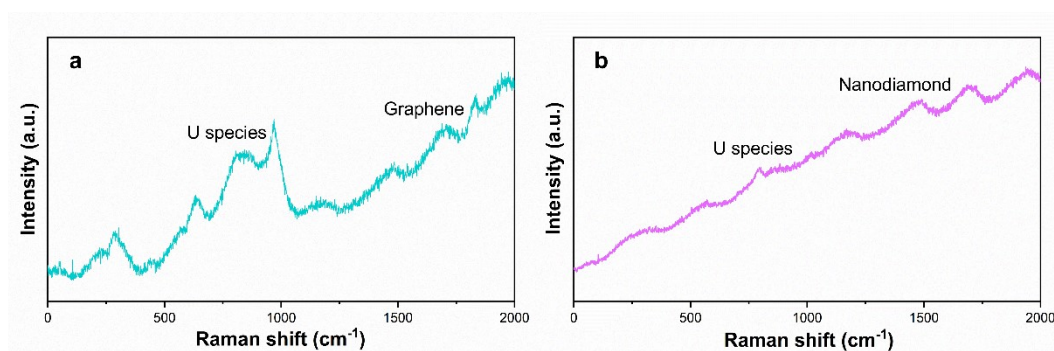


Figure S8: Raman spectra of uranium adsorption by (a): Graphene and (b): Nanodiamonds

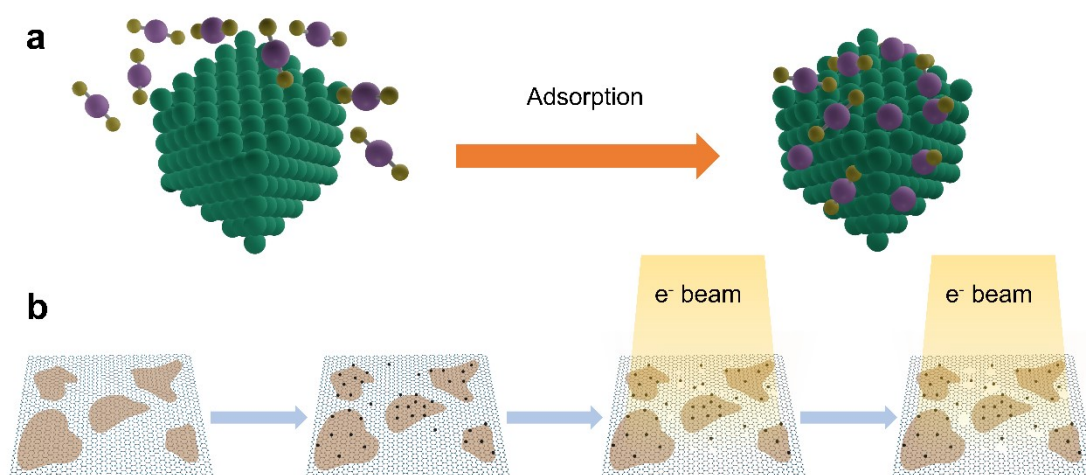


Figure S9: Schematic diagram of uranium adsorption by: (a) nanodiamond system and (b) graphene system.

Table S1: Relative mass content of elements after adsorption of uranium by carbonaceous materials analyzed by TEM eds mapping.

Material	C	N	O	U
Graphene	83.46	0.56	15.17	0.81
Nanodiamond	86.39	1.36	6.33	5.92

Table S2: Uranium interactions with different carbon allotropes

Material	Uranium Species	Binding Site	Irradiation Response
Graphene	Single atom	Hollow/top site of graphene/defects	Migration to edges/defects
Amorphous carbon	Single atom	Amorphous regions only	Limited migration
Nanodiamond	Uranyl ions	Oxygen-containing functional groups	No dissociation