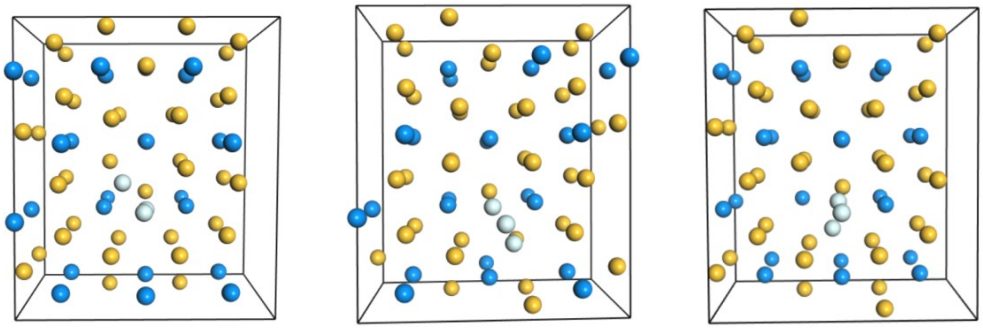
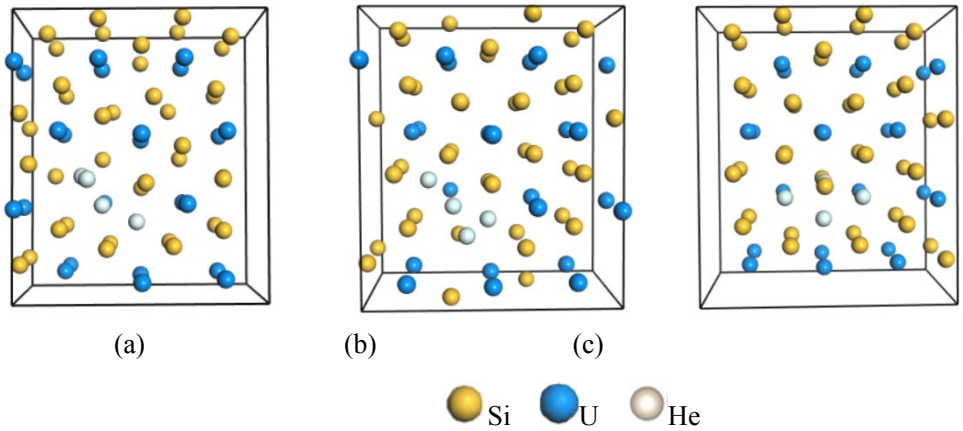
Electronic Supplementary Material (ESI) for RSC Advances.

Appendix A



(a) (b) (c)

Figure A1. The optimized structures of the secondary defects Nearest Si_1 (a), Nearest Si_2 (b) and Nearest U (c) associated with primary Si_2 vacancy and 3 He atoms.



(a) (b) (c)

Figure A2. The optimized structures of the secondary defects Nearest Si_1 (a), Nearest Si_2 (b) and Nearest U (c) associated with primary U vacancy and 4 He atoms

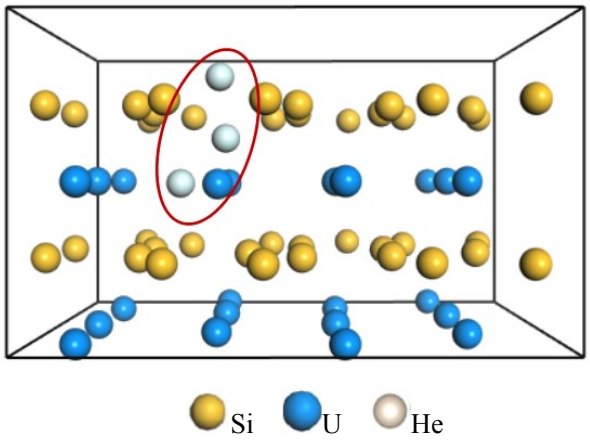


Figure A3. The optimized configure of 3 He atoms trapped in Si_2 vacancy.

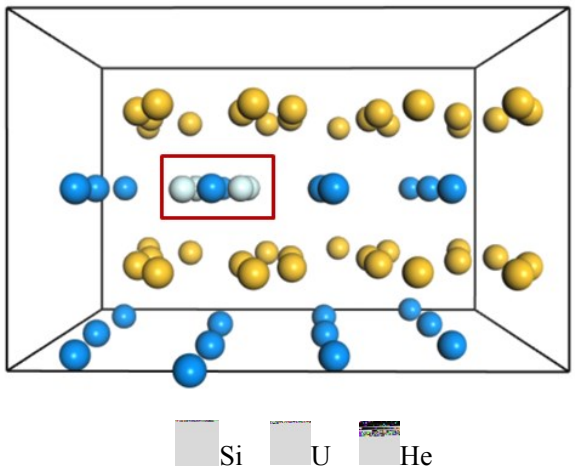


Figure A4. The optimized configure of 4 He atoms trapped in U vacancy.

Appendix A

Tab. A1 Lattice constant change and volume change associated with the He trapping in various interstitial sites

Structure	***a*(Å)**	***b*(Å)**	***c*(Å)**	***V*(Å^3)**	**Δ*a*/*a*(%)**	**Δ*b*/*b*(%)**	**Δ*c*/*c*(%)**	**Δ*V*/*V*(%)**
U_3Si_5	13.23	8.05	11.39	1213.60	0	0	0	0
1a	13.25	8.05	11.42	1218.85	0.15	0	0.26	0.43
3g	13.38	7.98	11.59	1237.74	1.13	-0.86	1.70	1.99
2c	13.11	8.29	11.31	1229.09	-0.91	2.98	0.70	1.28
6i	13.30	8.03	11.45	1223.89	0.57	-0.25	0.53	0.85