

Electronic Supplementary Information (ESI)

Atomistic Simulation of Helium Diffusion and Clustering in Plutonium Dioxide

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This supplementary information contains MSD plots of Pu, O and He at three temperatures for three supercell sizes (8x8x8, 10x10x10 and 12x12x12). It also contains visualisations of lattices with varying helium concentrations after molecular dynamics was run.

Table ESI.1: MSD of Pu, O and He in an 8x8x8 supercell at 1200, 2000 and 2800 K

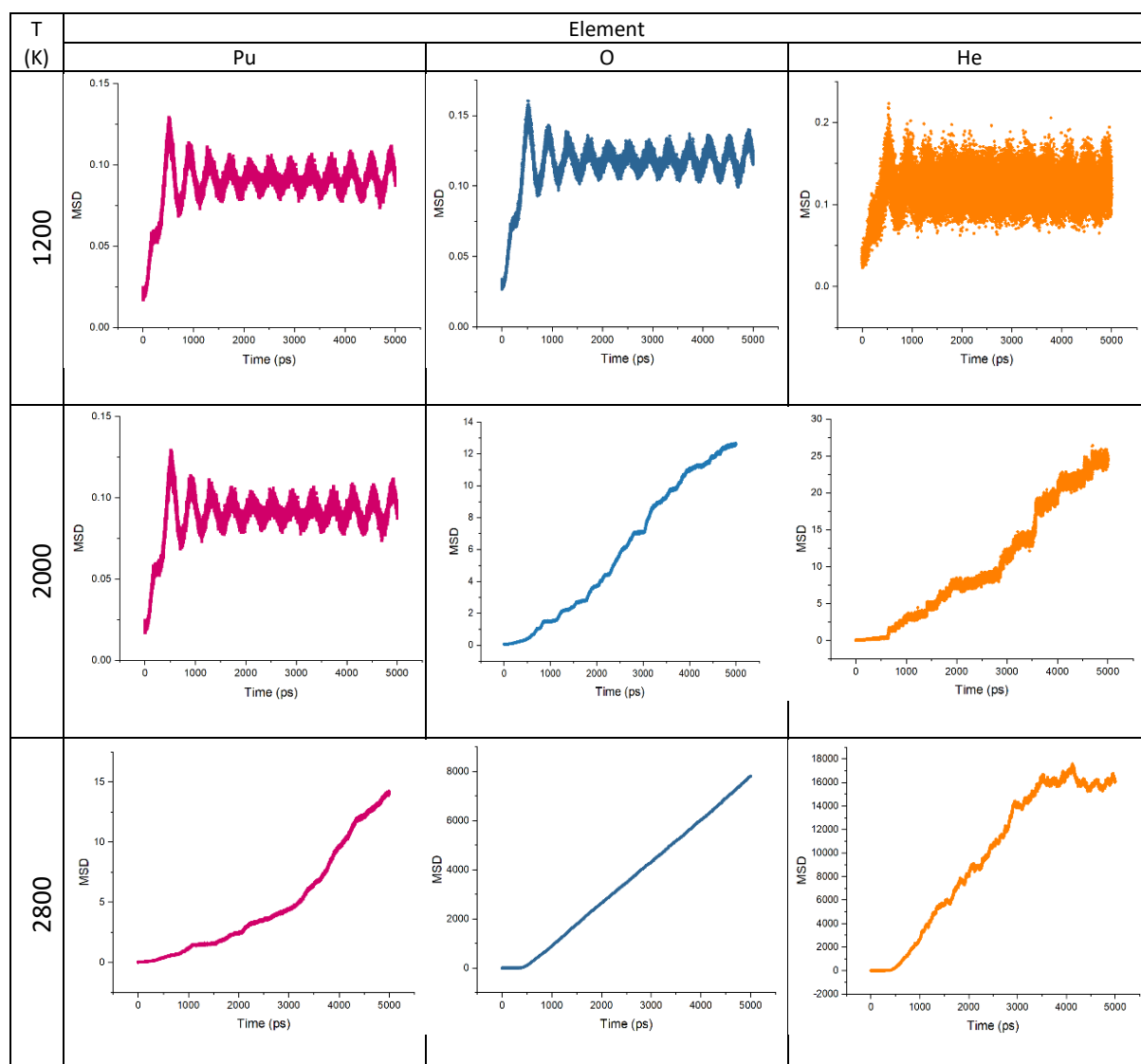


Table ESI.2: MSD of Pu, O and He in a 10x10x10 supercell at 1200, 2000 and 2800 K

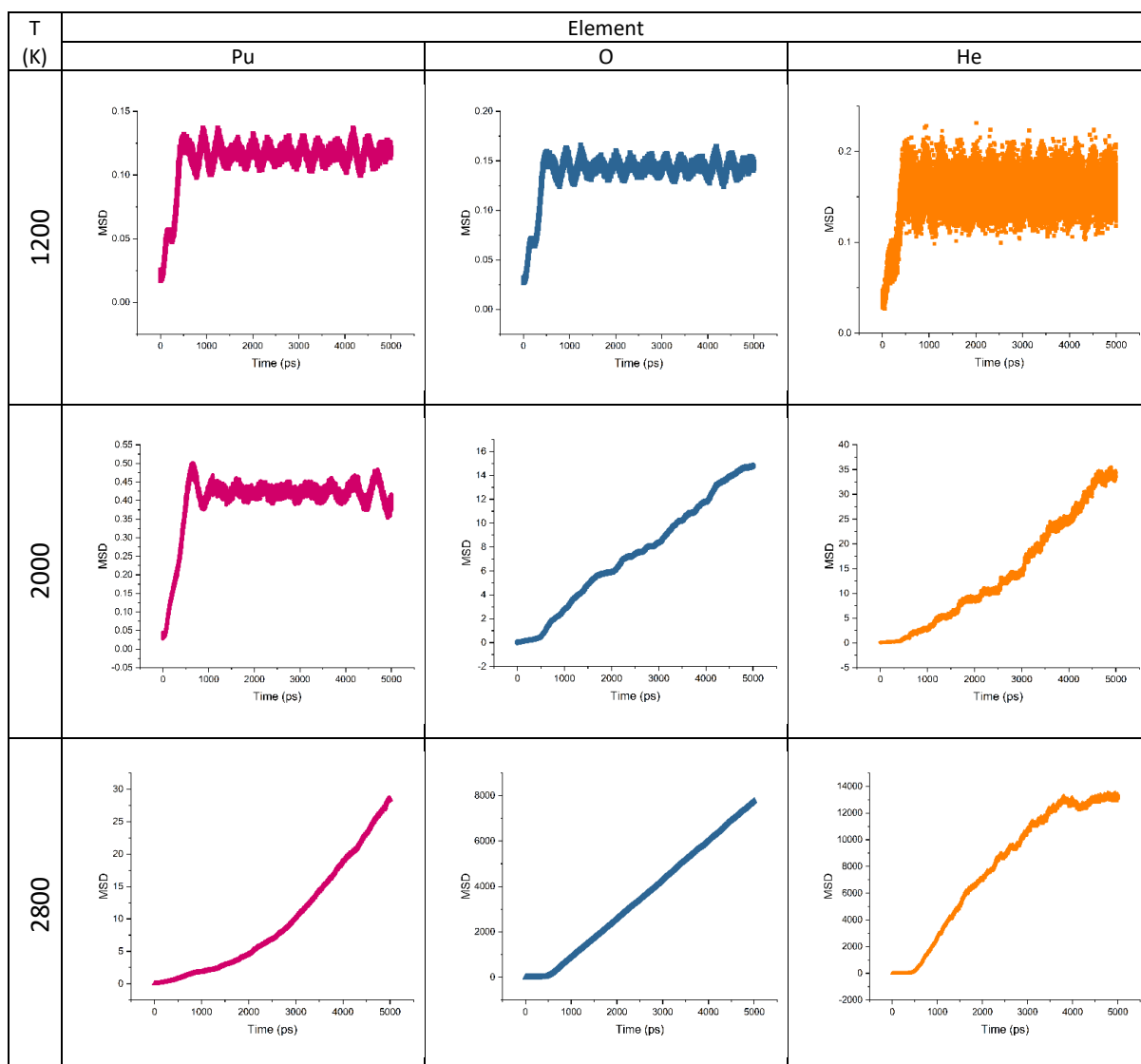


Table ESI.3: MSD of Pu, O and He in a 12x12x12 supercell at 1200, 2000 and 2800 K

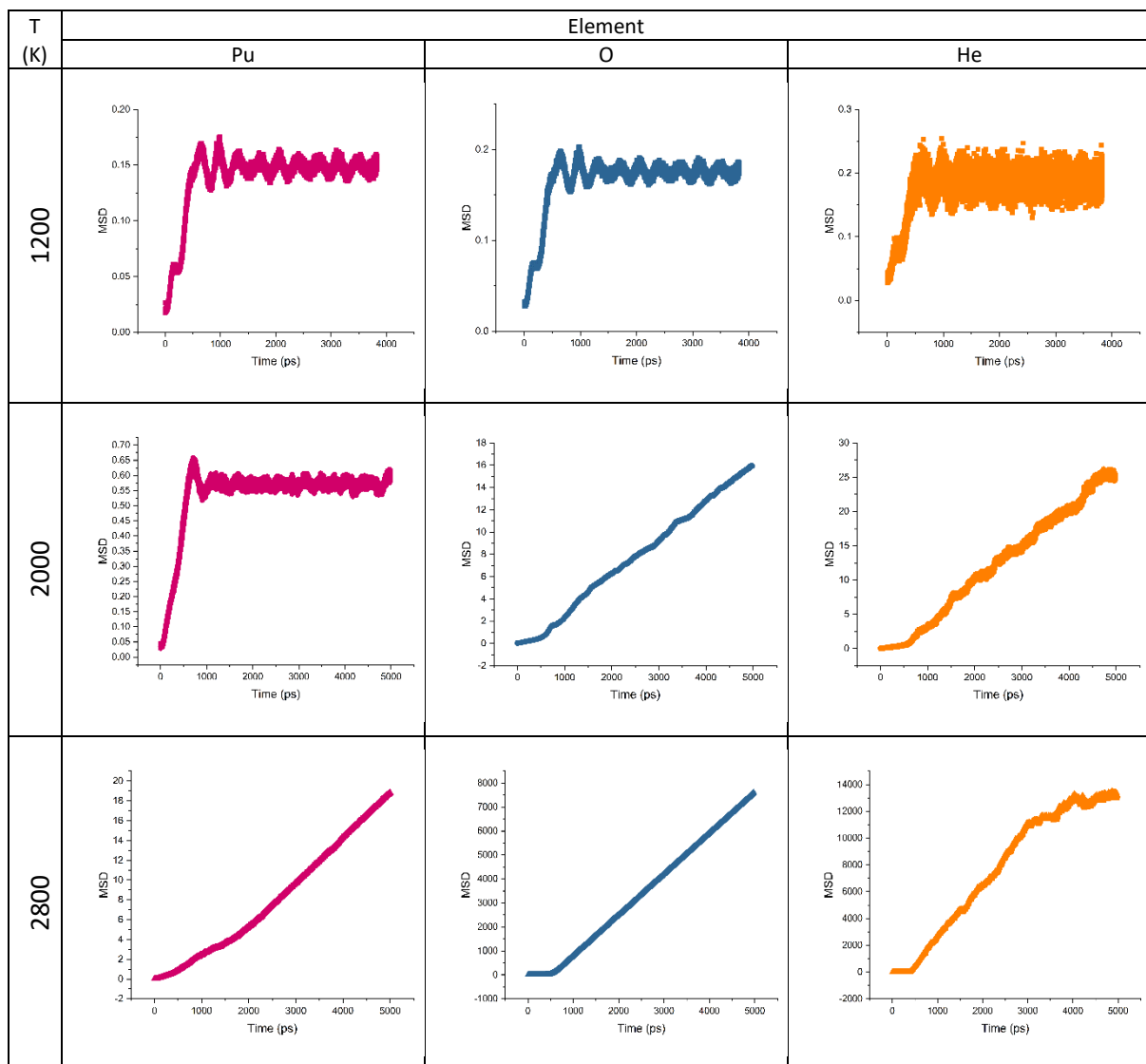
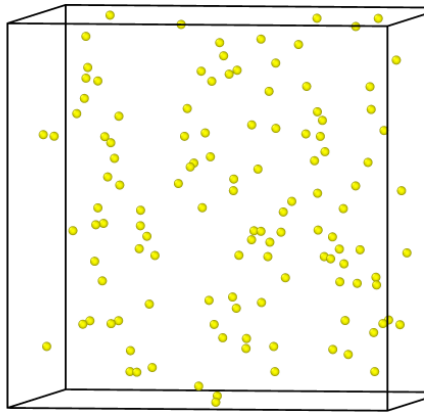
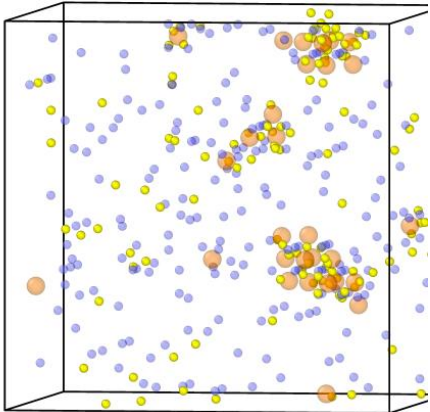
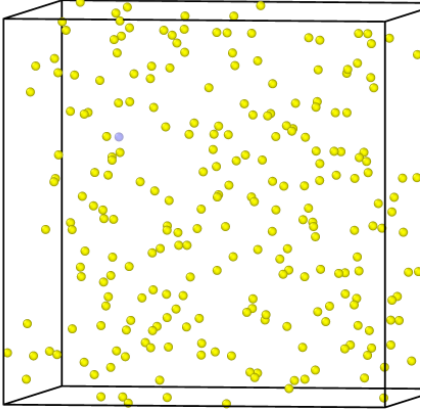
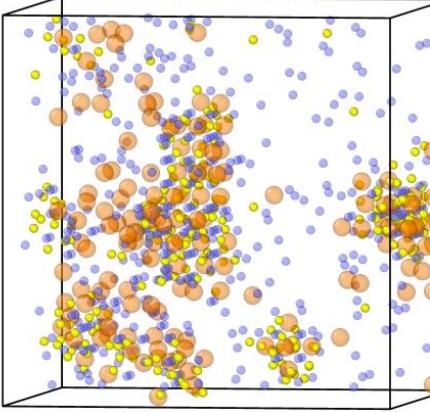
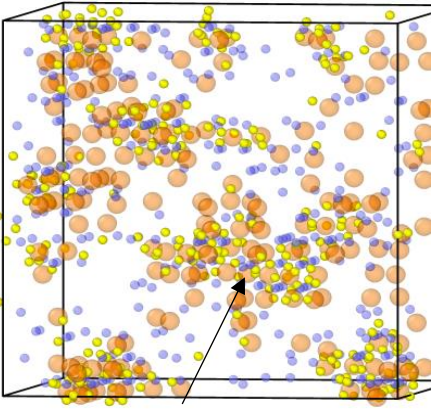


Table ESI.4: Visualisation of helium, oxygen vacancies and plutonium vacancies after 1 ns in PuO₂ at 2000 K (LHS) and 2500 K (RHS) at three different helium concentrations. For clarity, oxygen and plutonium ions are not displayed. It can be seen that at higher helium concentrations (10%), helium clustering occurs at lower temperatures. He is yellow spheres, O vacancies blue spheres and Pu vacancies pink spheres.

He Conc (wt.%)	Temperature (K)	
	2000 K	2500 K
2%	<p>0 He clusters</p> 	<p>3 He clusters</p> 
4%	<p>0 He clusters</p> 	<p>6 He clusters</p> 
10%	<p>15 He clusters</p>  <p>Helium trapped in a cluster at lower temp (2000 K) when concentration is higher (10%).</p>	<p>8 He clusters</p> 