

Title: Average structure and local configuration of excess oxygen in UO_{2+x}

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Supplementary information:

Figure S1: The atomic probability contour maps of U^{5+} (green) overlaid on the maps of U^{4+} (blue) and oxygen (red) projected on the (001) plane. U^{6+} atoms are not observed. As shown, at low temperature up to 800 K (a and b), the U^{5+} are localized near but not necessarily nearest neighboring to the interstitial oxygen atoms during the time scale of the simulations. Above 1200 K (c and d), the locations of U^{5+} are distributed over the most (c) or all (d) U lattice sites.

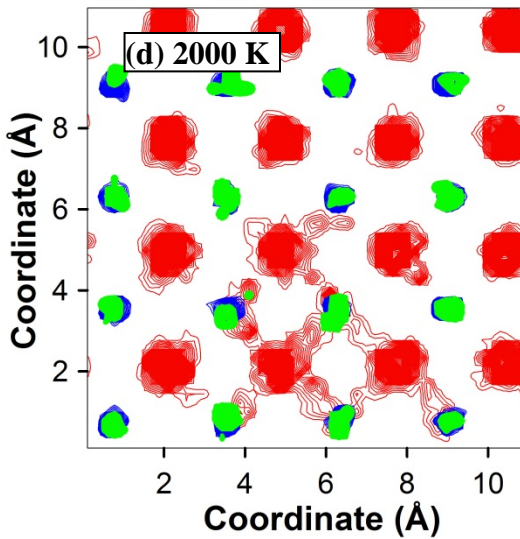
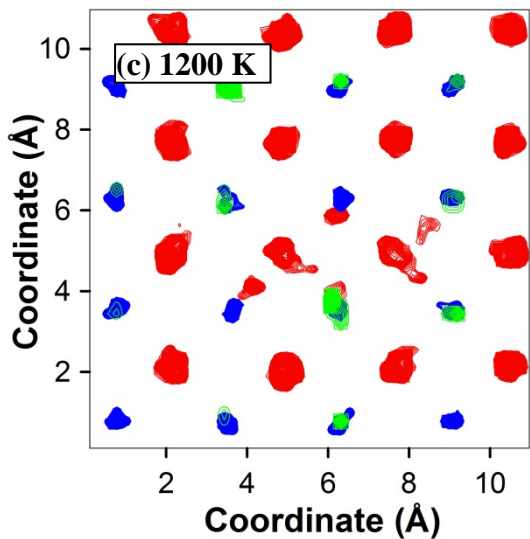
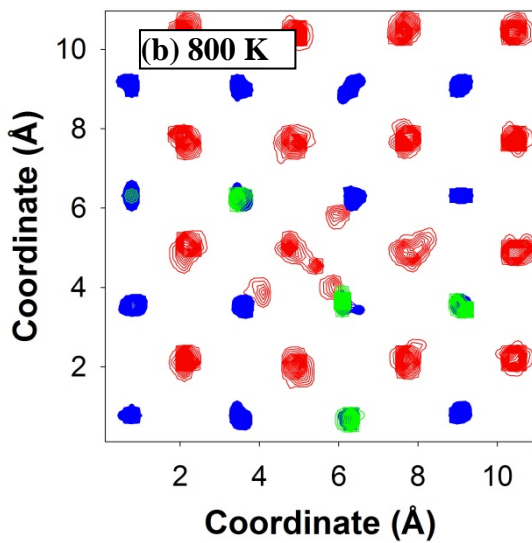
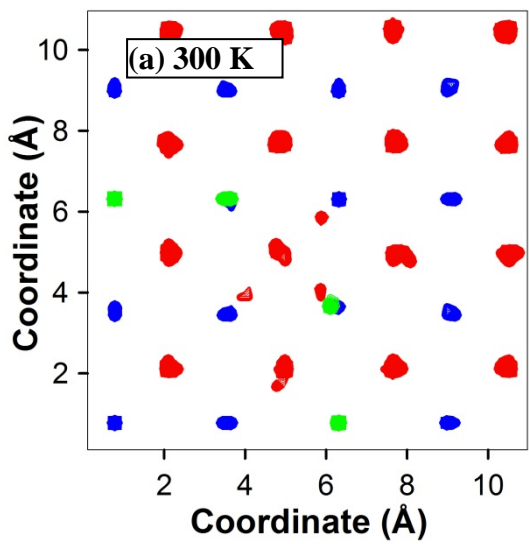


Figure S2: Probability distribution of the angle between $\langle 111 \rangle$ and the displacing direction of interstitial oxygen atom from the 4b site, averaged over the trajectory. Small values of angle are those interstitial oxygen atoms displaced in $\langle 111 \rangle$ directions and larger values are those in $\langle 110 \rangle$ directions. These distributions are used to calculate the ratio between $\langle 110 \rangle$ and $\langle 111 \rangle$ oxygen interstitials.

