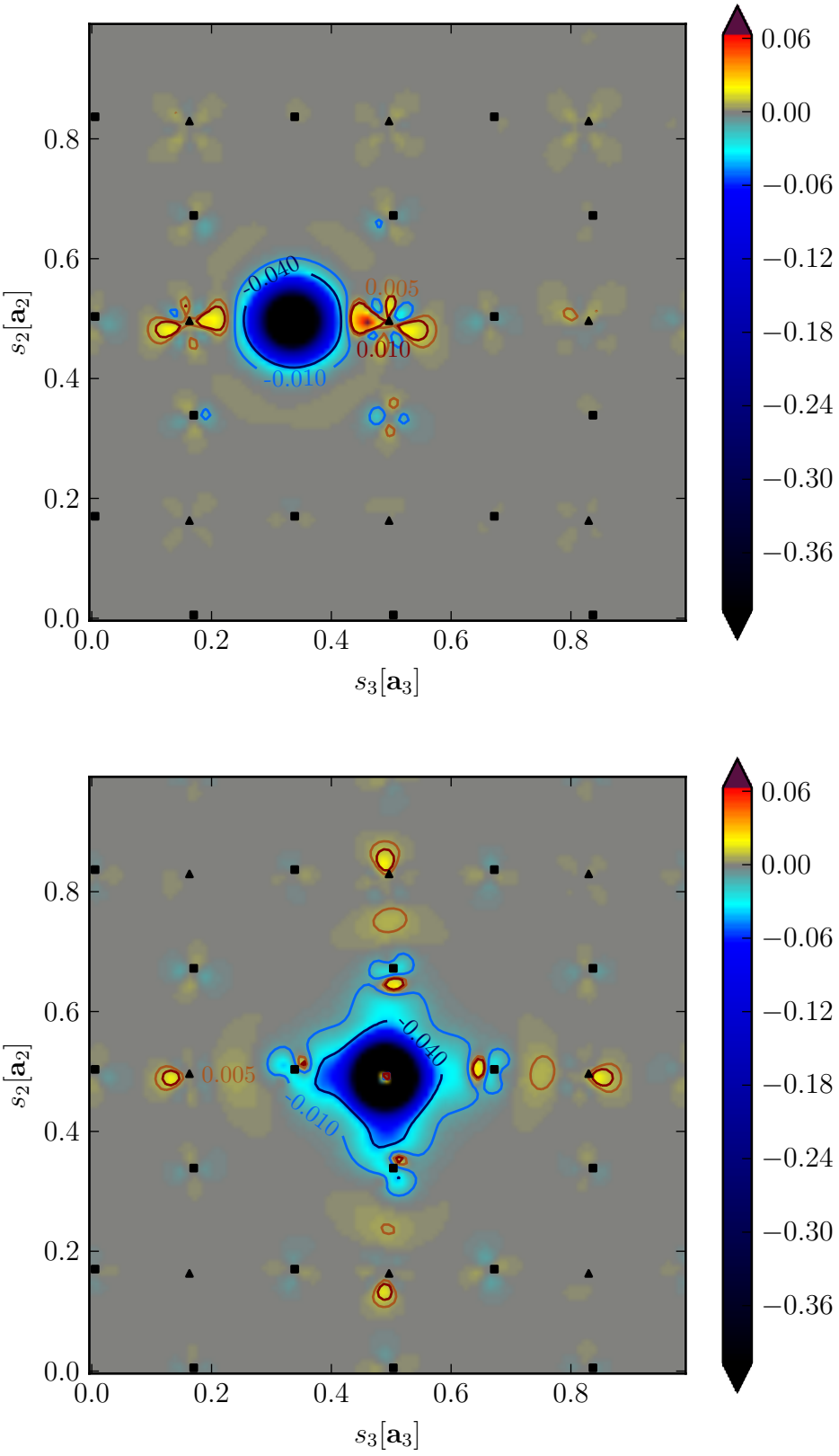

Figure 1: Electron number density difference $n^{\mathrm{V}}(\mathbf{r}) - n(\mathbf{r})$ where $n^{\mathrm{V}}(\mathbf{r})$ and $n(\mathbf{r})$ are the densities in the system with the vacancy and in the bulk, respectively. The Figure details and the colorbar scale are the same as in Fig. X.

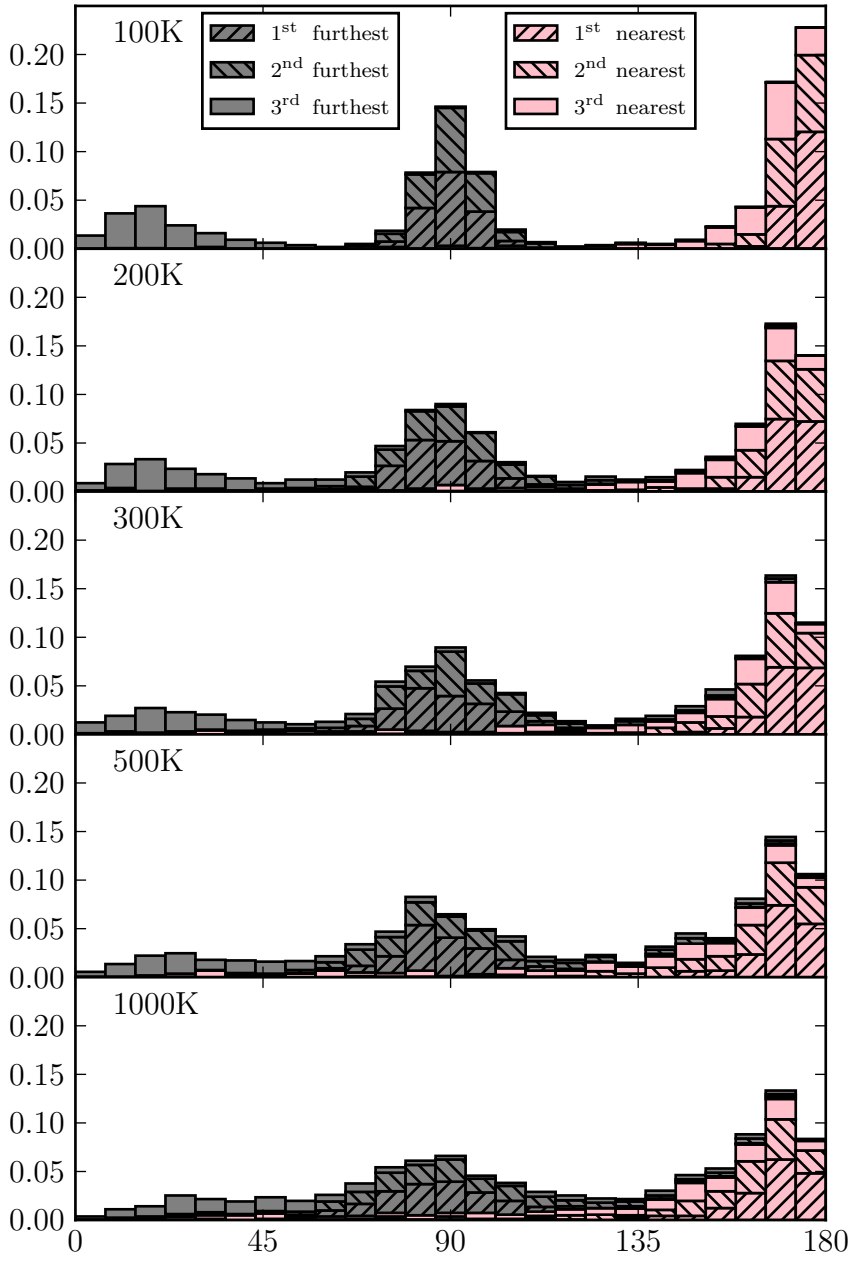

Figure 2: Normalised histogram of O dipole moment angles θ relative to nearest neighbour Ti ions, defined in text. For the three nearest O ions (pink) the dipole moments clearly point away from Ti at all temperatures.

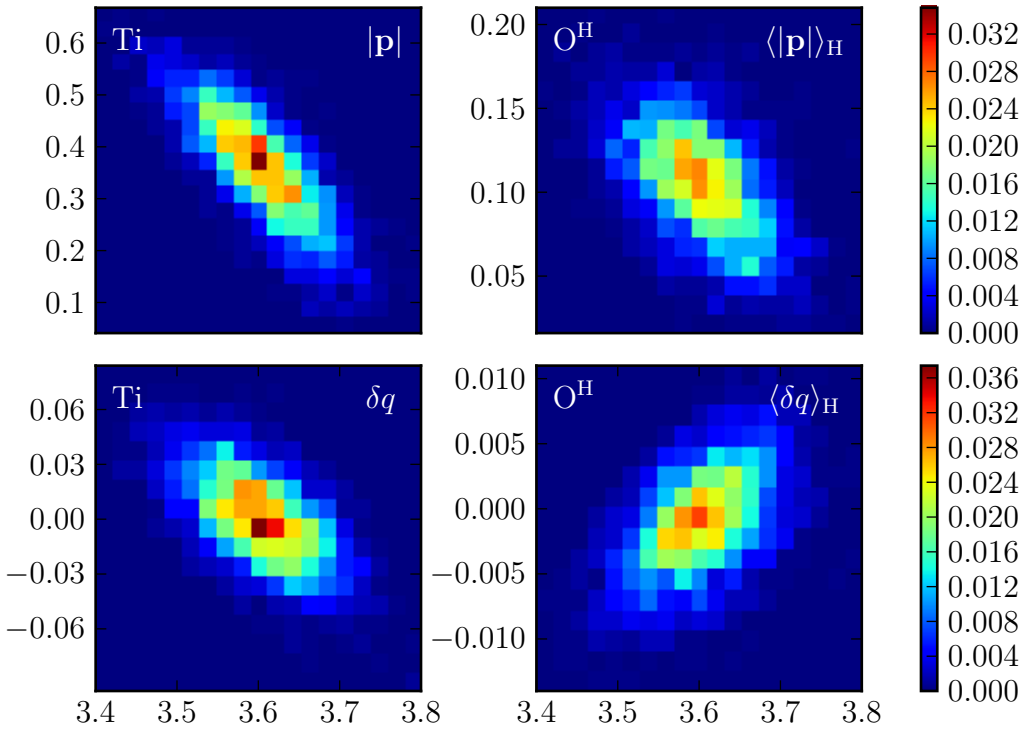

Figure 3: Dipole moment magnitude (top) and change in charge (bottom) on Ti ions (left) and averaged over three closest O ions (right). Histogram is from the 300 K NPH 100 ps MD simulation, configurations taken 1 ps apart.

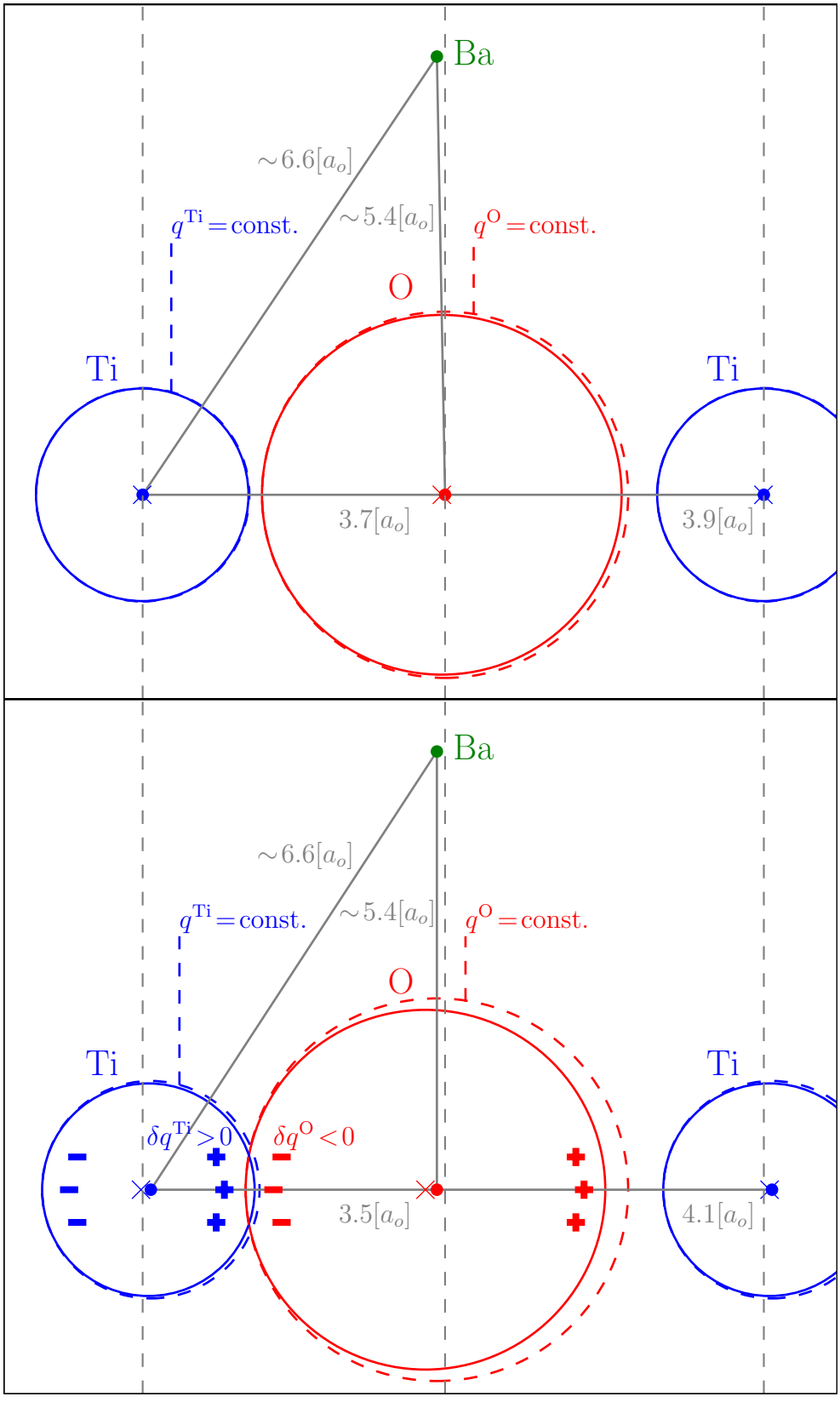

Figure 4: The × symbol indicates MLWFs' center-of-charge and the solid circle the size of the on-site electron cloud, as described in text. The dashed circles are centered at ionic nuclei, represented by solid dots, with the radius just large enough to enclose the solid circle. Dashed circles represent charge density of constant charge.