Supplemental Information

Oxygen vacancies in zirconia and their migration: the role of Hubbard-U parameters in Density Functional Theory

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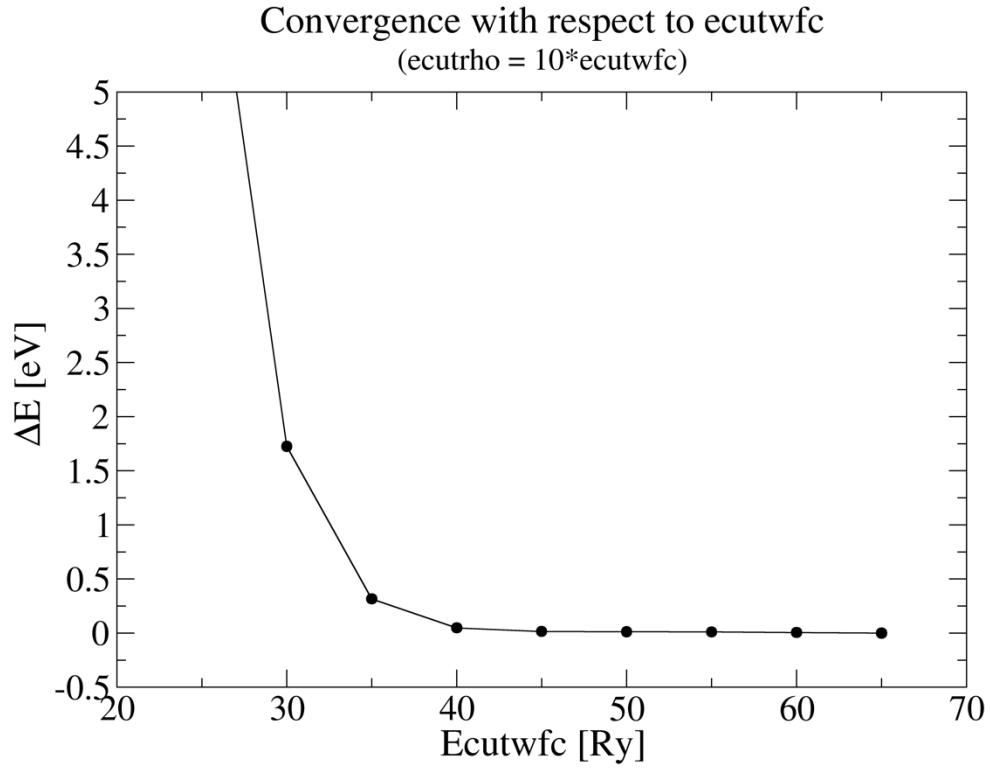
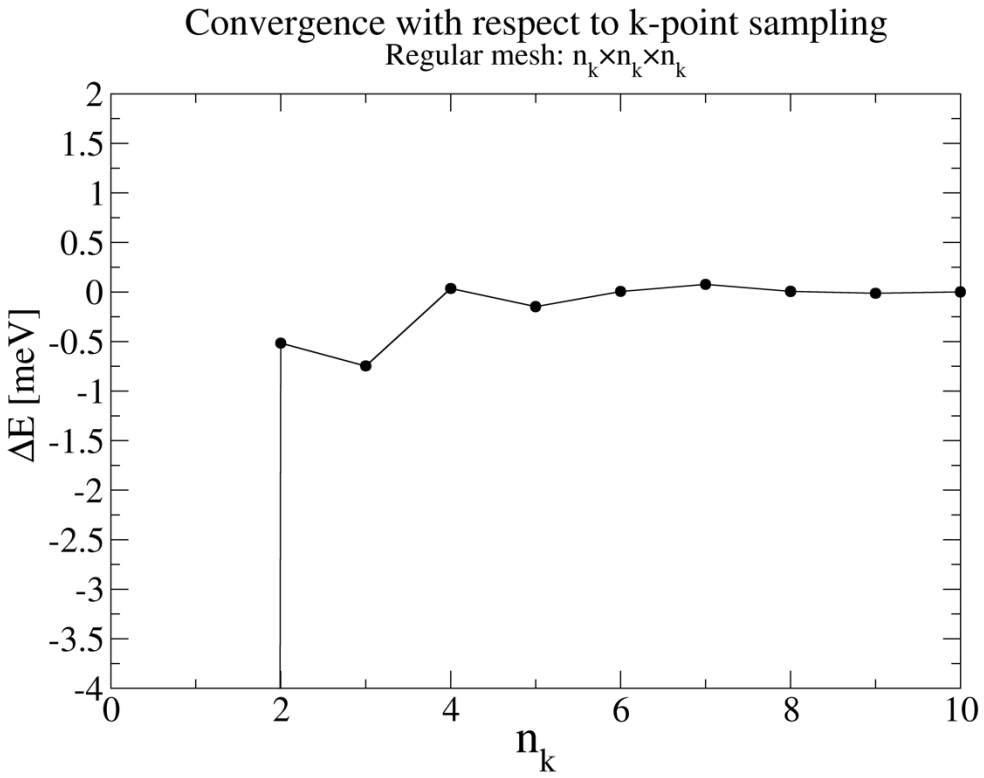
In the following we provide data regarding the convergence of the energy with respect to the basis set size and the k-point sampling. For the test, the 2×2×2 ZrO_2 supercell with 96 atoms was chosen. The total energy was calculated for the pristine system and the same system with one oxygen vacancy (95 atoms). The energy difference ΔE between the defected and the pristine system was calculated with varying values for the plane wave cutoff ecutwfc (ecutrho was set to 10×ecutwfc) and for the number of k-points. The Brillouin zone was sampled with a regular mesh of $n_k \times n_k \times n_k$ points. In the following graphs, the converged value of ΔE has been set to zero for clarity.
The calculations in the main paper have been performed with ecutwfc=40Ry (ecutrho=400Ry) and $n_k = 4$.




Convergence with respect to k-point sampling
Regular mesh: $n_k \times n_k \times n_k$
ΔE [meV]
n_k
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
-3
-3.5
-4
0
2
4
6
8
10