

Supporting information

“Influence of phase transitions and defect associates on the oxygen migration in the ion conductor $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$ ”

Kai-Christian Meyer and Karsten Albe

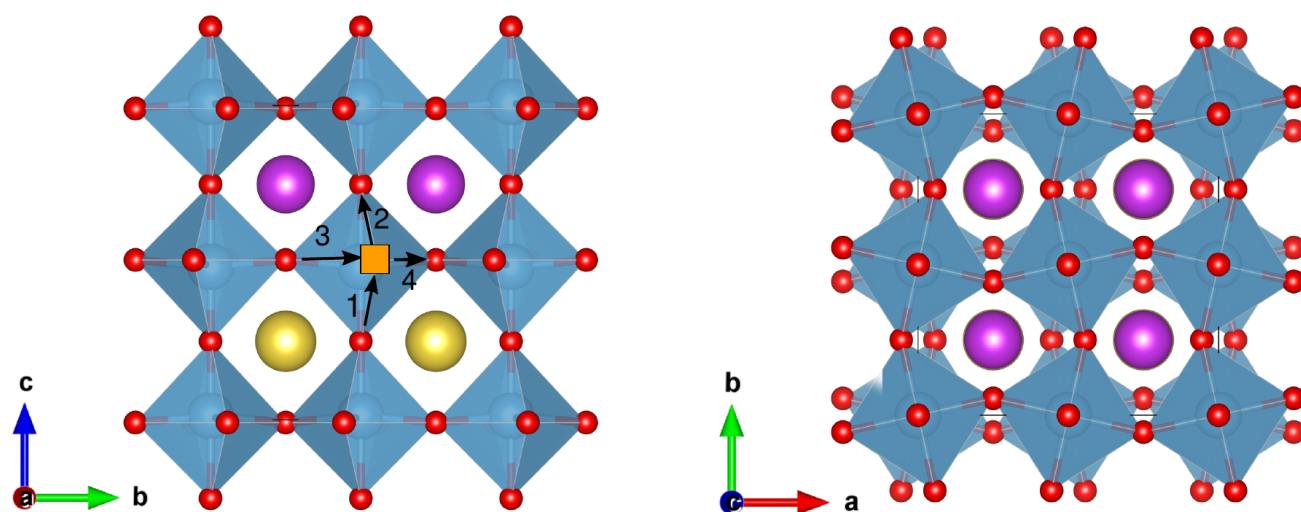


Figure S1 **Left:** Oxygen vacancy migration paths in the tetragonal structure. View along the [100]-direction. **Right:** The tetragonal structure viewed along the [001]-direction

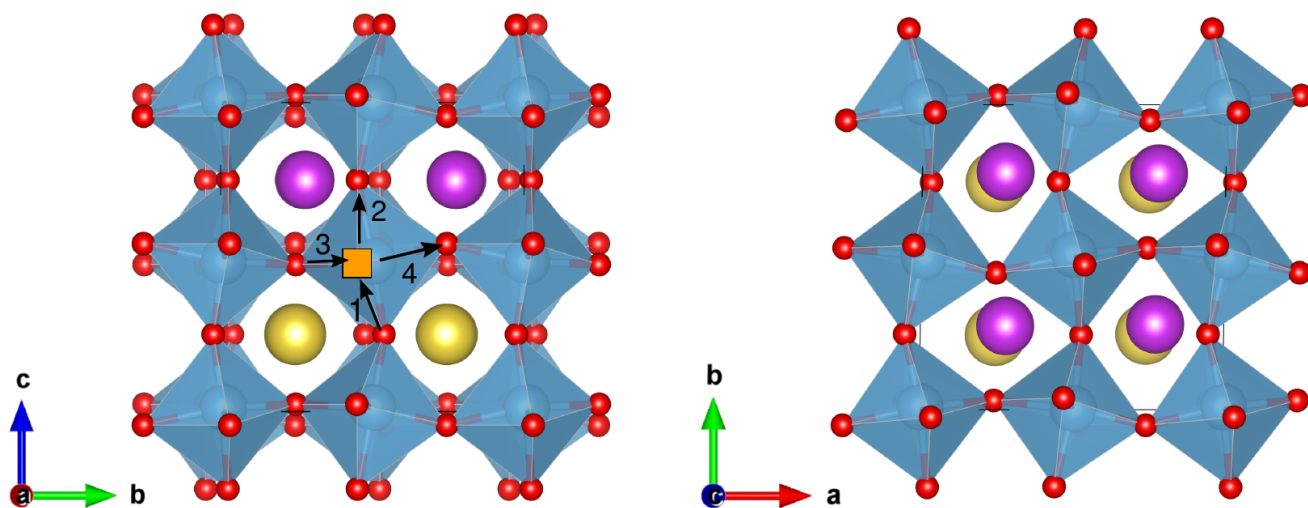


Figure S2 Left: Oxygen vacancy migration paths in the orthorhombic structure. View along the [100]-direction. Right: The rhombohedral structure viewed along the [001]-direction.

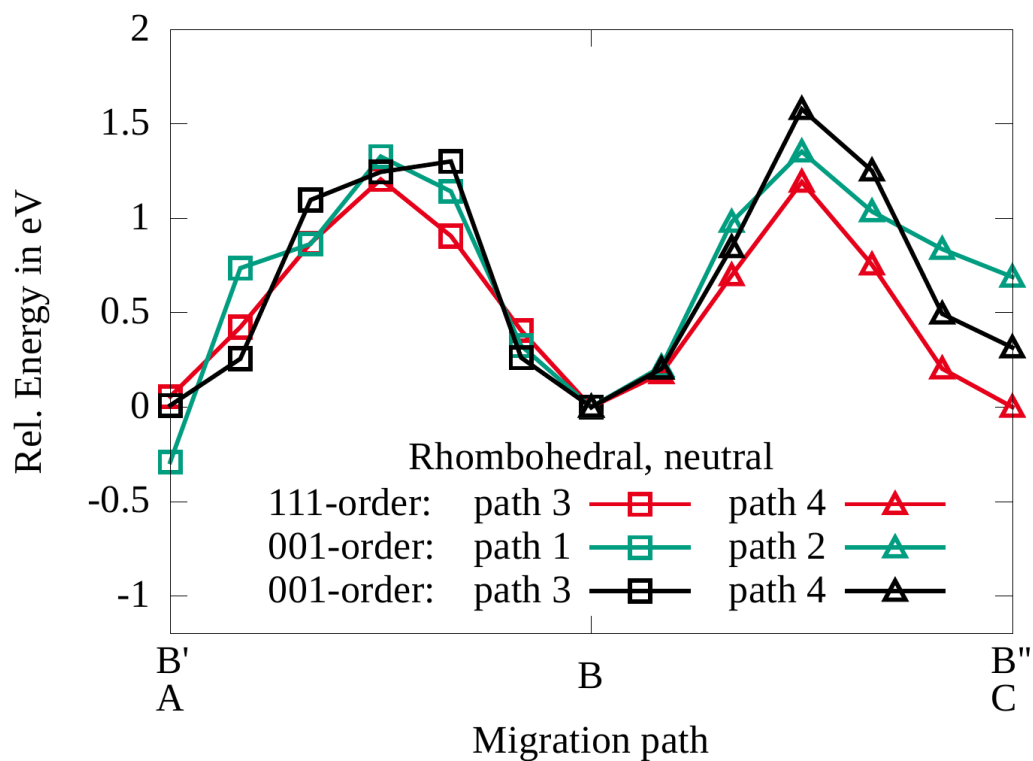


Figure S3 Oxygen vacancy migration barriers in the rhombohedral cell for the "neutral" case.

tetragonal structure II, path 4 (low barrier)

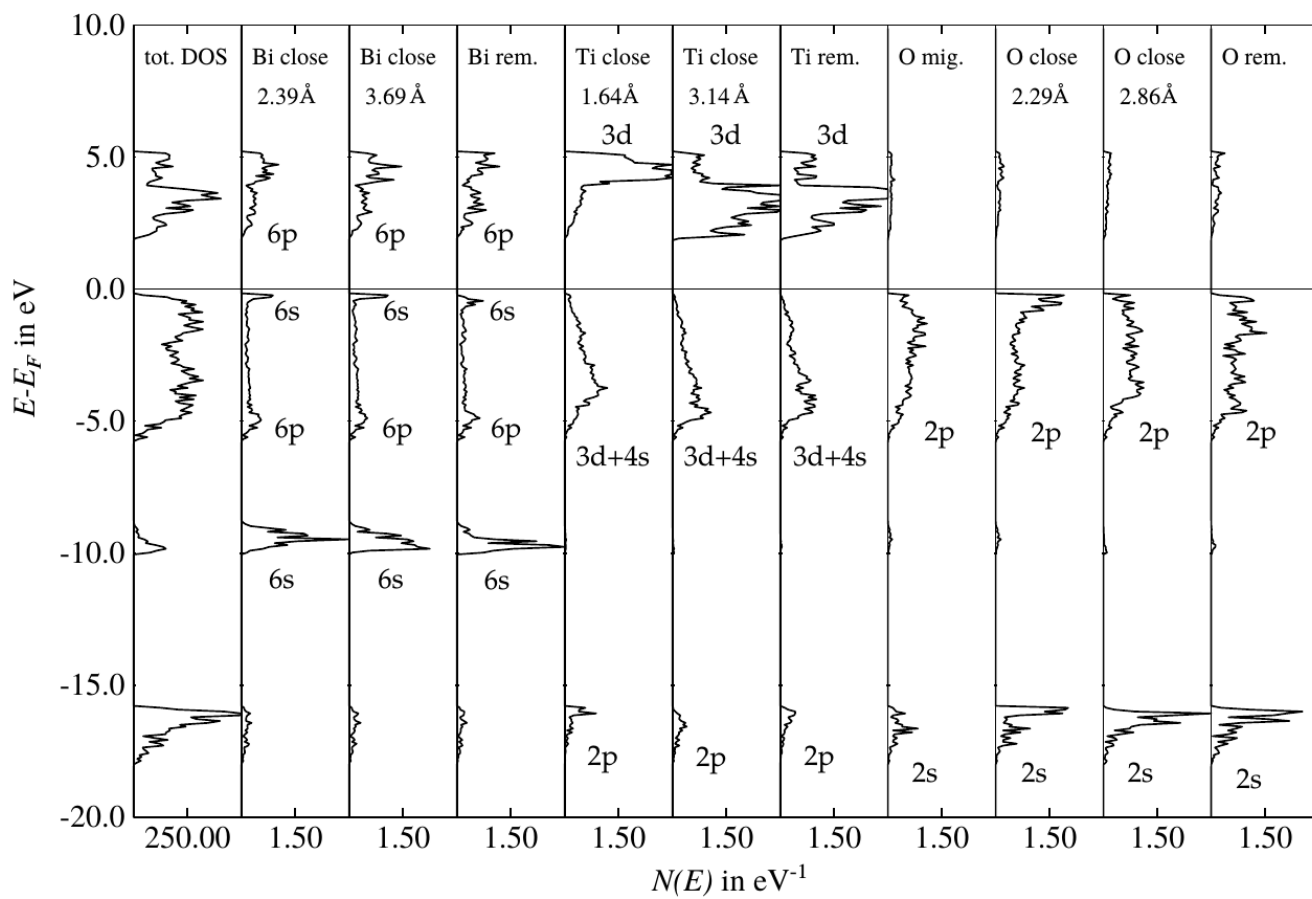


Figure S4 Electronic density of states of selected ions for the tetragonal structure II with a low migration energy barrier.