Electronic Supplementary Information

First-principles calculations of oxygen interstitials in corundum: site symmetry approach

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Our selected computational scheme very accurately reproduces the bulk properties of perfect corundum being used further in the calculations on oxygen interstitial atom behaviour therein performed using LCAO-DFT (B3PW) code CRYSTAL14.[1]

Table *SI*1 A comparison of calculated bulk properties of pure corundum crystal with the experiments. Phonon symmetry is given in parenthesis.

Properties	Expt.	LCAO-B3PW-CRYSTAL14
Cell parameter, Å	a = 4.759, c = 12.991[a] (ref. 47)	a = 4.761, c = 12.996
Band Gap, eV	9.3[b], 8.8[c]	8.72
Bulk modulus, GPa	253.7[d]	250.9
c_{44}, GPa	146.8[d]	156
Infra-red active frequencies, cm^{-1}	385,400, 442, 569, 583, 635[e]	397 (e_u), 409 (a_{2u}), 451 (e_u), 587 (e_u), 592 (a_{2u}), 648 (e_u)

[a] Ref. 2 [b] Ref. 3 [c] Ref. 4 [d] Ref. 5 [e] Ref. 6

Atomic configurations corresponding to Tables 1 and 2 of the main text are given below in Figures *SI*1,2

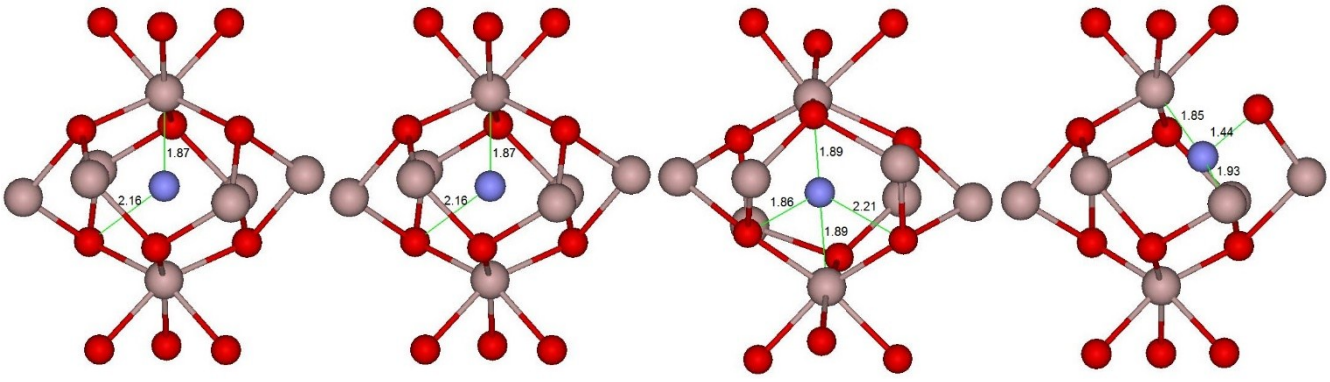
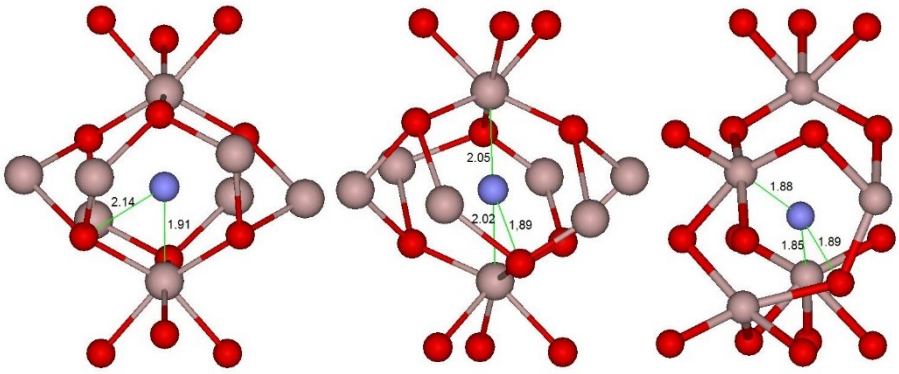


Figure *SI*1. Configurations of oxygen interstitials in different site symmetries in singlet state. Distances are given in Å.



*S*6/*S*3 *S*1 *S*2

Figure *SI*2. Configurations of oxygen interstitials in different site symmetries in triplet state. Distances are given in Å

References

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