Correction
Density functional theory study of superoxide ions as impurities in alkali halides

Sougaard Tygesen, Alexander ; Mathiesen, Nicolai Rask; Chang, Jinhyun; García-Lastra, Juan María

Published in:
Physical Chemistry Chemical Physics

Link to article, DOI:
10.1039/d0cp90113j

Publication date:
2020

Document Version
Publisher's PDF, also known as Version of record

Link back to DTU Orbit

Citation (APA):
Correction: Density functional theory study of superoxide ions as impurities in alkali halides

Alexander S. Tygesen, Nicolai R. Mathiesen, Jin Hyun Chang and Juan María García-Lastra*


In the right-hand column of the eighth page of the manuscript, all occurrences of the squared vibronic constant, $F$, should not be squared. Thus, the text should read: “The magnitude of the $Q_1$ distortion can be written in the first approximation as $Q_1^{\text{min}} = F/K$, where $F$ and $K$ are the vibronic coupling constant and the force constant for the $Q_1$ mode, respectively. In general, both $F$ and $K$ decrease as the lattice parameter is increased. It can be seen from Table 4 that the magnitude of the $Q_1$ distortion decreases as we move from sodium halides to potassium halides and from alkali bromides to alkali chlorides, which indicates that $F$ decreases faster than $K$ with the increase in lattice parameter.”

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.