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On the F-Centre in Calcium Fluoride

By

P. FELTHAM and I. ANDREWS

In a recent note Fleming (1) referred to our calculations of the F-centre absorption wavelength in calcium fluoride (2), suggesting that mathematical expediency may have led us to an incorrect choice of the lattice potential well. In the determination of the shape of the well, shown schematically as the full line 1 in Fig. 1, we utilised a scale model of the calcium fluoride lattice to find the approximate shape of curve 1 in the important volume of high charge density, contained within the fluorine vacancy, i.e. extending from the origin up to about r_F in Fig. 1. On going in the [111] direction singularities occur on the well surface at sites of the calcium and fluorine "point" ions, a section through the well is represented by the dashed curve.

The problem of determining a well shape suitable for continuum treatments of colour-centre absorption wavelengths is well known (3, 4) and we did not consider it necessary to indicate or discuss the discontinuities, here shown on the dashed curve, specifically, depicting only the part lying between the origin and the nearest calcium ion, corresponding to the branch denoted by curve 2 in Fig. 1.

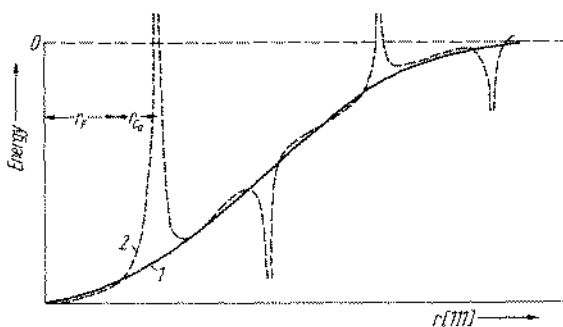


Fig. 1

Fleming appears to be under the erroneous impression that this branch of the dashed curve should be taken as the lattice potential rather than our curve 1. It is obvious that such a mistaken assumption must lead to a gross underestimate of the 1s-2p transition energy of the F-electron, as, in fact, he finds to be the case.

References

- (1) R.J. FLEMING, phys. stat. sol. 13, K87 (1966).
- (2) P. FELTHAM and I. ANDREWS, phys. stat. sol. 10, 203 (1965).
- (3) S.R. TIBBS, Trans. Faraday Soc. 35, 1471 (1936).
- (4) J.H. SIMPSON, Proc. Roy. Soc. A 197, 269 (1949).

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