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STUDY OF A POSITIVE HYDROGEN ION IN CRISTALLINE Si

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Abstract: Energies and wave-functions of an isolated proton in a Si crystal are calculated. The results indicate that in the ground state the proton is essentially localized in the interbond regions.

1. Method

The behaviour of an isolated proton in a Si crystal is studied by approximating the particle-host interaction with an effective potential which neglects lattice-distortion effects. The potential was calculated [1] with a linear response scheme based on density functional theory in the local density approximation [2,3] and using the non-local pseudopotential method [4]. The periodic Schroedinger equation for the proton is then solved in terms of a Bloch-like basis set obtained by linear combinations of gaussian orbitals centered on the minima of the effective potential and the C, M, hexagonal and antibond sites. The gaussian widths are used as variational parameters. The large basis set (72 Bloch states) guarantees good convergence of both energies and wave-functions: increasing the basis set dimension from 60 to 72, the change in ground state energy is 0.1 meV and that of the wave-function maximum is 0.4%. Comparable accuracy is obtained for a number of low-energy excited states.

2. Results

The ground state of the proton is at Γ with energy -8.21 eV relative to the average value of the effective potential which is assumed as zero. The lowest 11 excited states at Γ are

nearly degenerate with the ground state (the largest excitation energy is 7 meV). A second group of levels (36 states) has energies ranging between 0.05 eV and 0.12 eV above the ground state, while a third group (16 states) has energies between 0.32 eV and 0.40 eV and is well separated from higher states. It is interesting to compare the ground state energy of the proton with those of the deuteron (-8.25 eV) and positron (-5.26 eV) calculated in a previous work [5]. The proton density in the ground state is given in Fig. 1. The figure clearly shows that the proton is strongly localized in the potential minima which occur all around the bond centers.

3. References

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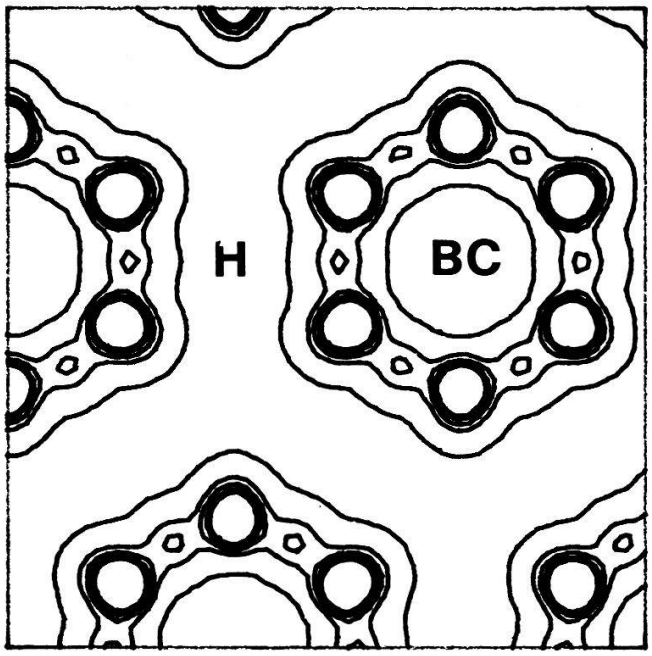

Fig.1 : Contour plot in the (111) plane passing through the bond centers of the proton density in the ground state (in units of particle per cell). The lowest contour is at 0.05 and adjacent contours are separated by 1.5. The density peaks correspond to the potential minima which occur slightly off-plane.