

crystal Hamiltonian and a term corresponding to the point defect. This difference ( $H'$ ) is a localized function centered about the  $F^-$ -vacancy. The wavefunction of the  $F^-$ -center electron is expanded in terms of symmetrized linear combinations of orbitals centered at various shells of atoms near the  $F^-$ -vacancy. Multicenter integrals involving  $H'$  are evaluated using the Gaussian method. A similar numerical technique is also utilized for determining the effects of lattice relaxation due to the presence of the  $F^-$ -center. The results of the ground state  $F^-$ -center calculation yield the charge density around the defect which is used to obtain an improved potential function. A description of the wavefunction and energy of the  $F^-$ -center electron will be presented.

FF 3 Search for Zero-Phonon Line of  $F_2$ -centers in KCl. J. ROLFE and S.R. MORRISON, N.R.C., Ottawa, Canada.--The  $F_2$  (M) center in KCl has a multiphonon absorption band at 8000Å and a multiphonon emission band at 10,600Å. A zero-phonon line should lie between these; calculation of its expected position from the parameters of the multiphonon absorption band places the line at 8245Å, and a similar calculation from emission band parameters gives 9115Å. A search was made with a sensitive absorption apparatus capable of measuring  $10^{-4}$  change in transmittance with a band-pass of 0.8Å, using KCl crystals at 2°K. These crystals had aligned  $F_2$  centers with an absorption optical density of 6 in the  $[1\bar{1}0]$  direction and an optical density of 2 in the  $[110]$  direction. No zero-phonon line with the required anisotropic absorption was found in the wavelength region 8000-11,000Å, though 42 isotropic zero-phonon lines were detected in a Harshaw KCl crystal with aligned  $F_2$  centers. These isotropic lines are probably caused by impurities, since in a similarly treated Optovac crystal no zero-phonon lines at all could be detected.

FF 4 Pseudopotential Calculations of F Center Wavefunctions and Hyperfine Interactions in NaCl and KCl. ROBERT J. FRIAUF and SOO-UNG KIM, U. of Kansas.--A potential including modified Slater exchange<sup>1</sup> and non-local pseudopotentials is obtained from mutually orthogonal crystal ion wavefunctions<sup>2</sup> for 6 shells of ions around an F center. Very good agreement for optical absorption energies and oscillator strengths indicates a good fit for both the size and shape of wavefunctions obtained from this potential. Calculated isotropic hfs constants are good to 10% for shells 1 and 2 but small by 30% for shells 5 and 6. Anomalies at shells 3 and 4 are only partly accounted for by our results. The extended ion treatment of Wood<sup>3</sup> gives slightly poorer results for shells 1 and 2 but better results for shells 3 and 4. Exact calculations of amplification factors show variations as large as 50 to 100% for different ion positions and crystals. Thus accurate hfs constant calculations require adequate treatment of all core orbitals and also careful attention to the orthogonality of these orbitals.

<sup>1</sup>R.J. Friauf and S.U. Kim, Bull. APS 18, 473 (1973).

<sup>2</sup>R.J. Friauf and S.U. Kim, Bull. APS 19, 372 (1974).

<sup>3</sup>R.F. Wood, Phys. Stat. Solidi 42, 849 (1970).

FF 5 A New Interstitial Hydrogen Defect in Alkali Halides.\* S. MORATO† and F. LUTY, Univ. of Utah--Hydrogen atoms in neutral ( $H^0$ ) and negative ( $H^-$ ) form on substitutional and interstitial sites are well studied model defects in alkali halides ( $U$ ,  $U_1$ ,  $U_2$ ,  $U_3$  centers). A new stable form of interstitial hydrogen has been discovered, with no pronounced electronic absorption, but a single sharp local mode band (at  $1114\text{ cm}^{-1}$  in KCl). Hydrogen in this form can be produced by a variety of processes: UV photo-decomposition of  $OH^-$  and  $SH^-$  defects at LNT, U photo excitation at LNT, thermally or optically stimulated reaction of  $Cl_2^-$  crowdions ( $H$  centers) with  $H^-$  Frenkel pairs, and prolonged x-irradiation of crystals with U cen-

ters at LNT. The local mode shows a perfect  $\sqrt{2}$  ( $H \rightarrow D$ ) isotope shift; its strength and single structure indicate a charged hydrogen in a symmetric position. Extensive experiments on the production and destruction suggest as model a  $H^-$  in body-centered interstitial position with a trapped hole shared by the four equivalent  $Cl^-$  neighbors. This defect corresponds to a charge-transfer excited state of the  $U_2$  (interstitial  $H^0$ ) center, apparently stabilized by a strong Jahn Teller distortion.

\*Work supported by NSF Grant #GH43353X.

†Fellowship from FAPESP. Now at IEA, São Paulo, Brasil.

FF 6 Local Phase-Transitions From Off- to On-Center Defects Under Hydrostatic Pressure.\* U. HOLLAND and F. LUTY, Univ. of Utah--The tuning of shallow off-center  $Cu^+$  and  $Ag^+$  defects into on-center positions by hydrostatic pressure can be monitored by the strength of the weak parity-forbidden ( $d+s$ ) UV transitions, which become stronger (partially allowed) by the odd-parity off-center distortion. After preliminary studies of  $Ag^+$  in RbCl and RbBr, reported earlier, a new system ( $NaBr:Cu^+$ ) was found and extensively studied. It displays a single UV band at RT which becomes accompanied by a second band of similar strength when cooled below 90K. Hydrostatic pressure reduces both these absorptions (by more than a factor of 10 at 4K), indicating an off-center  $\rightarrow$  on-center transition of the  $Cu^+$  ion. Contrary to a simple theoretical model, the absorption does not change gradually at LHeT, but shows an abrupt decrease at a critical pressure, characteristic for each defect system. This favors the picture of a "local phase transition" from off- to on-center behavior. Corresponding dielectric measurements under pressure, aimed at detecting directly the dielectric contribution from the off-center dipoles, are under way; first results of this new technique will be reported.

\*Work supported by NSF Grant #GH43353X.

FF 7 Color Center Formation and Radioluminescence in NaCl, KCl, and LiF Measured During and After Electron Bombardment.\* P.W. LEVY, K.J. SWYLER, and W.H. HARDY, II, Brookhaven National Lab.--Recently, equipment has been completed for simultaneous measurement of optical absorption and luminescence of samples during continuous electron bombardment. Typically, separate 256 point absorption and luminescence spectra, covering 200 to 400 or 400 to 800 nm, are recorded every 40 sec. 1.5 MeV, 50 nanoamp irradiation at room temperature causes both color center formation and radioluminescence. In LiF, the emission occurs in a single strong band near 3.0 eV which increases with dose. NaCl shows several pronounced emission bands which decrease with dose, while in KCl several very weak bands occur which appear to decrease with dose. F-center absorption grows rapidly to saturation in NaCl and KCl, but continues to increase monotonically in LiF. When the irradiation is terminated, radioluminescence ceases, and very little phosphorescence is observed. F-center stability varies greatly after irradiation. In LiF and NaCl the F-center concentration does not decay rapidly, in KCl marked decay is observed. The F-center growth kinetics are simple in KCl and NaCl, but complex in LiF.

\*Work supported by the U.S. Atomic Energy Commission.

FF 8 Absorption and Luminescence Measurements on Glasses During Continuous Electron Irradiation.\* K.J. SWYLER, W.H. HARDY, II, and P.W. LEVY, Brookhaven National Lab.--Apparatus for simultaneously recording optical absorption and luminescence during electron irradiation has been used to study coloring in soda-lime-silica (NBS710), lead-silica (NBS711), and lanthanide (AO-C) glasses. All three glasses develop strong absorption bands at 3 to 4 eV and weaker bands at 1.5 to 2 eV. The high energy band is approximately 15 times greater than the low energy band. Typically, 50 na/cm<sup>2</sup> 1.5 MeV irradiations ( $5 \times 10^3$  rad/sec) produce "saturation" coloring in  $4 \times 10^3$