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Molecular orbital calculations based on the Extended Huckel Theory have been performed for clusters of two and eight SiO, molecules. We report here the results for an ordered structure in which periodic boundary conditions are imposed to saturate the peripheral bonds which otherwise cause extraneous localized states to appear. We find an energy gap of ~ 13 eV as compared to the experimental value of $\sim 11\,\text{eV}$. The removal of an oxygen results in several levels in the energy gap which move upon displacement of the two neighboring silicons. The levels appear to account for the observed ultraviolet optical absorption band and are also a possible origin for the positively charged slow surface states present near a SiO₂-Si interface. The addition of either atomic or molecular hydrogen to a perfect crystal is predicted to yield preferentially a double hydrogen-single oxygen center. If ambient oxygen atoms are present, a two hydroxl group center is then most favorable.

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5. LATTICE DYNAMICS OF CUBIC ZINC SULFIDE BY NEUTRON SCATTERING

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The dispersion properties of room temperature cubic ZnS were measured in high symmetry directions by the constant-Q method. A valence shell model, following the method of Woods et al., was least square fitted to the neutron data with only fair success. This model and its comparison with a rigid ion version are discussed. Longitudinal optic branches were not observed.

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6. TRANSPORT ANOMALIES IN DILUTE SILVER-RARE EARTH ALLOYS

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It is noted that the residual resistivities for Ag alloyed with rare earth impurities from the latter half of the rare earth series are approximately three times the residual resistivity for any other trivalent impurity. Moreover, these residual resistivities are essentially independent of the magnetic character of the impurities. New thermoelectric power data indicate the impurity contributions to the diffusion thermoelectric power are positive. These anomalies are shown to be consistent with a very simple model which includes core contributions to the scattering.

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7. THE OPTICAL SPECTRUM AND MAGNETIC PROPETIES OF TmFeO₃ IN THE SINGLE-ION MODEL

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The optical absorption spectrum of trivalent thulium in the orthoferrite is reported as a function of temperature, magnetic field, and photon polarization. Transitions are shown to be electric dipole. Singlet states of the ground multiplet are found at 0, 17.5, 39, and 70 cm⁻¹; their representation labels, characteristic of the low symmetry C_{1h} site of the thulium ion, are A', A', A'', and A'' respectively. The form of the single-ion Hamiltonian matrices describing the applied and molecular field perturbations on these crystal field states is derived and is used to account for Zeeman splittings. The size of molecular field interactions is estimated from the breakdown of selection rules. Single-ion contributions to the temperature-dependent magnetization and anisotropy are derived on the basis of the optical data and are shown to be compatible with experiment.

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