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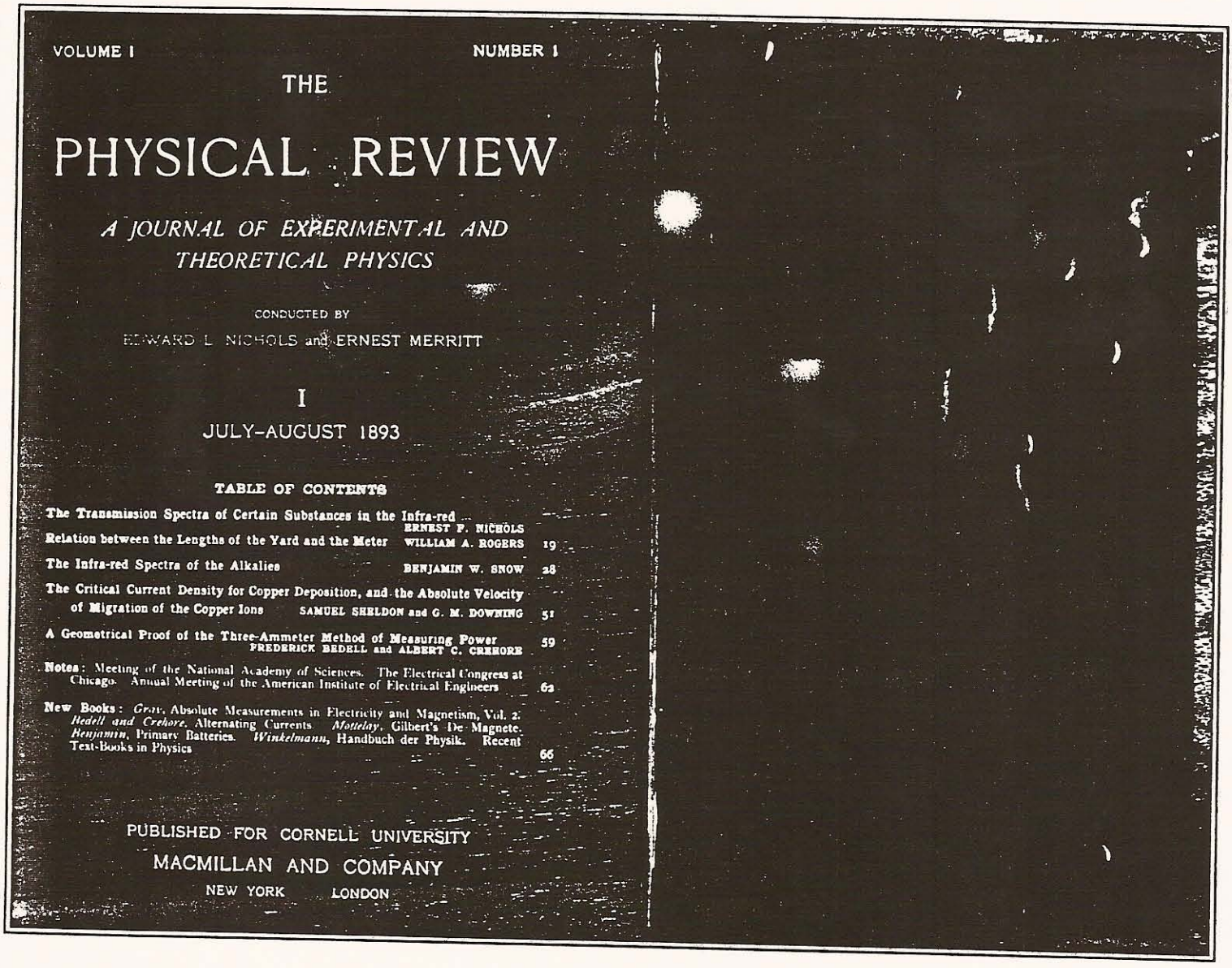

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SESSION E11: MOLECULES, CLUSTERS, AND OPTICAL TECHNIQUES

Tuesday morning, 13 April 1993
Room 15 at 8:00
E. Eyler, presiding

8:00
E11 1
Homonuclear Metallic Nanoclusters : Structure and Energetics . C. W. Finley, Penn State University, New Kensington, Pa. 15068, P. Abel, and J. Ferrante , NASA Lewis, Cleveland, Ohio 44135. We have calculated the energy and equilibrium geometry of Ni, Pd, Pt nanoclusters ($N \leq 16$) using the Universal Binding Energy version of the Embedded Atom Method. We find that the fit of the average binding energy of the atoms in the clusters to

$$E = \alpha\,(4\pi/3)\,R^3 + \sigma\,4p\,R^2 + \gamma\,2\pi\,R,$$

when α and γ are the fitting parameters, is excellent.

8:12
E11 2 Effect of Substrate Temperature on UV laser Induced Si Ion Emission From Si(100) Surface. H.T. Liu and Z. Wu*, Dept. of Phys., Rutgers Univ. — We study the Si ion emission from Si(100) surface under the irradiation of low flux 193 nm pulsed laser beam from an excimer laser. Ions were detected using Time-of-Flight technique. The identity of Si ions was verified by checking the isotopic ratio of mass 28 and mass 29 counts. A large unexpected temperature effect was observed for the ion yield. As the temperature of the substrate increases, the yield of Si ions initially increases and reaches a maximum at about 800 K and then decreases as temperature further increases. One possibility is that the emission of Si ions is related to the kinks on type S_B steps, which are known to become more numerous as temperature increases. The decrease of ion yield at higher temperature is not understood. Precautions were taken in the experiment to make sure that (1) the absorption of the incident laser beam was the same for different temperatures and (2) while data were being taken, the heating current was momentarily stopped and the substrate was at ground potential.

* Supported by NSF grant DMR-9022134

8:24
E11 3 Dynamical Fragmentation of Multiply Charged Clusters.. E. BLAISTEN-BAROJAS, N. BAKALTCHEV, CSI and Physics Department, George Mason University.--- The process of symmetric versus non-symmetric fragmentation of multiply charged atomic clusters consisting of several hundreds of atoms was studied by molecular dynamics. The potential energy surface of the fragmentation process is calculated for various sizes of clusters and the results compared to the liquid drop model originally applied to the nuclear fission problem. Time changes of the polarizability and of the cluster shape deformation are responsible for transient energy barriers that affect the fragmentation channels. Critical sizes for multiply charged clusters are determined. The degree of delocalization of the charge distribution plays an important in the fission pattern. Evaporation of single atoms is also observed and the energetics between fragmentation and evaporation is discussed.

8:36
E11 4 Near-threshold continuum structure and the dissociation energies of H_2, D_2, and HD.* E.E. Eyler, B. Catching, and N. Melikechi, University of Delaware.--- The vibrational continuum adjoining the $H(1s) + H(2l)$ dissociation limit has been investigated with a resolution of 0.01 cm^{-1} by double resonance through the EF state. In this extension of our earlier work,[1] the continuum is detected both by multiphoton ionization and by a separate Balmer-α laser that ionizes the $H(2s)$ or $H(2p)$ dissociation products. We observe both the continuum onset and fine-grained structure above it due to interferences and shape resonances. The near-threshold continuum is usually dominated by dissociation to $2s$ atoms, although non-adiabatic mixings lead to substantial $2p$ atom production in at least one case. The dissociation energies can be determined from the continuum onsets with an accuracy of about 0.05 cm^{-1}. The results agree well with theory and other recent measurements. However, measured linewidths of C state shape resonances disagree with calculations by Burciagga and Ford.[2]

*Supported by the National Science Foundation.
[1]E. F. McCormack and E.E. Eyler, Phys. Rev. Lett. 66, 1042 (1991).
[2]J.R. Burciaga and A.L. Ford, J. Mol. Spect. 149, 1 (1991).

8:48
E11 5 A Possible Test of the Pauli Exclusion Principle in Spherical Top Molecules. K. FOX, U Tennessee and U Maryland - Rotational-vibrational transitions in the electronic ground state of molecules with tetrahedral symmetry are examined to determine experimental conditions for a possible test of the Pauli exclusion principle. The connection between nuclear spin and statistics is particularly significant for the tetroxides of ruthenium and osmium in which the zero spins appear to exclude, completely, certain states in these molecules. Laser transitions coincident with related Pauli forbidden states are calculated. Competing effects, including those from excited vibrational states, are considered. The connection between the principles of parity conservation and Pauli exclusion in these experiments is also explored.

9:00
E11 6 Computed Vibrations in the Ar-N_2 Complexes. Z. SLANINA, MPI Chemie, S.J. KIM, ST Systems and K. FOX, U Maryland and U Tennessee - Harmonic vibrations in the Ar-N_2 complexes are computed ab initio using the second-order Moller-Plesset (MP2) perturbation treatment with the 6-31G* basis set; the energetics are refined at the MP4 fourth-order level. Two different minimum-energy structures are found, T-shaped and linear; the latter being lower in energy. The intersystem vibrations exhibit 30 cm^{-1} or lower frequencies. The intramolecular N_2 frequency is lowered by about 0.4 cm^{-1} compared to a free N_2 molecule. The highest infrared intensity is found for the intramolecular mode in the T-shaped structure. Results are relevant for spectroscopy of planetary atmospheres.

9:12
✶ **E11 7** Vibronic and Rotational Analyses of LIF Spectra of CH_3O and CH_3S Radicals. P. MISRA, X. ZHU, H. BRYANT, A. NUR, and M. KAMAL, Howard Univ. --- Several vibronic bands belonging to the $\tilde{A}$-$\tilde{X}$ system of methoxy (CH_3O) and methylthio (CH_3S) radicals have been recorded in the near UV under low (0.2 cm^{-1}) and high (0.07 cm^{-1}) resolution in a cold supersonic jet environment. Wavelength-resolved emission spectra have also been obtained by dispersing the laser excited fluorescence with a 0.6 m monochromator having a resolution of 0.3 nm. A comprehensive analysis has provided information regarding the ground