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Electronic structure and dynamics of elements at high pressures¹

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Electronic structure and dynamics information of materials under high pressure has been very scarce due to the experimental difficulties. The standard electronic probes using electron energy loss spectroscopy (EELS) is limited to vacuum pressures. The optical probes that can reach high-pressure samples through the diamond windows, on the other hand, are limited by the energy accessibility (< 5 eV) and near-zero momentum transfer, $q = (4\pi/\lambda_0) \sin \theta$. These problems can be overcome by the newly advanced, two-photon, inelastic, x-ray, scattering (IXS) spectroscopy which uses high energy xrays ($\sim 10^4$ eV) to provide the atomic-level momentum transfer and to enter (with energy E) and exit (with energy E_0) the pressure vessel. The electronic spectra are revealed by analyzing the x-ray energy loss between the two photons, $\hbar\omega = E - E_0$. Using IXS facilities at third-generation synchrotron source, we studied electronic structure and dynamics of two elements at high pressures in a diamond-anvil cell: i.e., He, the widest-gap insulator, and Na, the archetypal free-electron metal. At 11.9-17.9 GPa in a single crystal ^4He , we observed rich electron excitation spectra, including a cut-off edge above 23 eV, a sharp exciton peak showing linear volume dependence, and a series of excitations and continuum at 26 to 45 eV. We determined electronic dispersion along the 100 direction over two Brillouin zones, and provided a quantitative picture of the helium exciton beyond the simplified Wannier-Frenkel description. At 1.6-4.39 GPa in a polycrystalline Na sample, we observed the sharp plasmon peak at low q and its dispersion beyond the critical q_c . The plasmon shifts to higher energy under compression and drastic reduction of r_s . *Ab-initio* theoretical calculations are conducted for interpretation of the experimental results.

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