

Abstract Submitted
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Persistence of Covalent Bonding in Liquid Silicon Probed by Inelastic X-ray Scattering JUNPEI OKADA, Japan Aerospace Exploration Agency (ISAS/JAXA), P. SIT, Princeton U., Y.J. WANG, B. BARBIELLINI, Northeastern U., Y. WATANABE, U. Tokyo (JAPAN), A. BANSIL, Northeastern U., Y. SAKURAI, JASRI/SPring-8 (JAPAN), M. ITOU, JASRI/SPring-8, T. ISHIKAWA, ISAS/JAXA, K. KIMURA, U.Tokyo, P. PARADIS, ISAS/JAXA, S. NANA0, U.Tokyo — Metallic liquid silicon at 1787K is investigated using x-ray Compton scattering. An excellent agreement is found between the measurements and the corresponding Car-Parrinello molecular dynamics simulations. Our results show persistence of covalent bonding in liquid silicon and provide support for the occurrence of theoretically predicted liquid-liquid phase transition in supercooled liquid states. The population of covalent bond pairs in liquid silicon is estimated to be 17% via a maximally-localized Wannier function analysis. Compton scattering is shown to be a sensitive probe of bonding effects in the liquid state.

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