

■ ASSOCIATED CONTENT

SI Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.jpcllett.1c04090>.

Includes the procedures and methods for the preparation of the bromine- and amine-treated HPHT ND samples with the debromination studies under open-air and inert conditions using DRIFTS. XPS analysis and model for determining surface coverage of chemical groups. N 1s XAS control samples, X-ray beam damage, and amide bond formation control experiments. Explanation and analysis of the suppression of the diamond core–hole exciton after ND–Br reactions with propargylamine. Resonant X-ray inelastic scattering maps taken for various chemical preparations of the HPHT NDs ([PDF](#))