Canadian Association of Physicists
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Contribution ID: **250** Type: **Oral Competition (Graduate Student) / Compétition orale (Étudiant(e) du 2e ou 3e cycle)**

Theoretical Insights into Hydrogen-Encapsulated Cage-like Structure and the Elusive High-Pressure Electride of Na-tI50 phase.

Monday 9 June 2025 15:00 (15 minutes)

Advances in science and technology rely on new materials and molecules with tailored chemical, mechanical, electronic, and superconducting properties. The development of reliable quantum-mechanical approaches has accelerated progress in the discovery of new materials. This is largely owing to the rapid progress of computer power and theoretical methods, particularly density functional theory (DFT) and machine-learned assisted structure prediction methods. Indeed, these computational techniques and theoretical models pave the way for establishing the structure–property relationship for designing advanced materials with novel properties and improving their performances. Using first-principles density functional calculation, we integrated molecular hydrogen into a boron-carbon clathrate framework, and our study reveals a hydrogen-encapsulated hole conductor with an estimated superconducting transition temperature (Tc) of 46 K and dynamically stable at ambient pressure, highlighting it as a candidate for next-generation technologies. Furthermore, by combining a machine learning-assisted structural search with density functional theory (DFT), we successfully resolve the elusive high-pressure tI50 phase of sodium and predicted it to be a high-pressure electride. These findings highlight the unique structural, electronic, and dynamic behaviors of these materials, offering transformative insights into superconductivity and high-pressure physics.

Keyword-1

Density Functional Theory

Keyword-2

Superconductivity

Keyword-3

Machine learning Potential

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