

Aromaticity, Closed-Shell Effects, and Metallization of Hydrogen

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Scientific Achievement

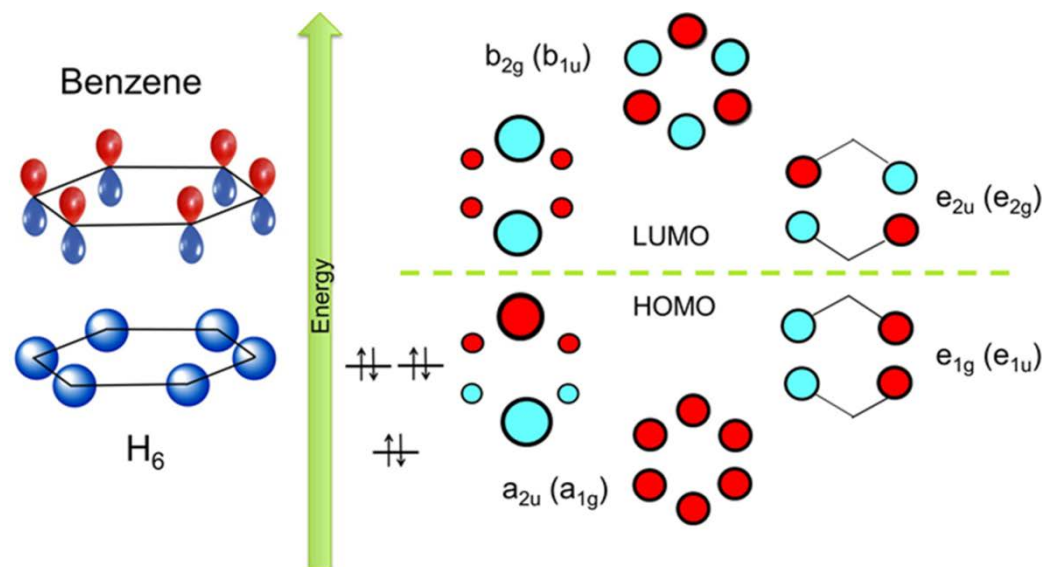
The atomic and electronic properties of dense hydrogen at very high pressures are controlled by closed-shell effects that parallel those of graphene

Significance and Impact

The results are essential to understanding of how the dense hydrogen becomes metallic – the state predicted to have exotic properties including high- T_c superconductivity

Research Details

- Hydrogen in different forms - molecular clusters, 2D and 3D crystals – was studied using modern quantum chemistry and solid state approaches.
- The stability of dense hydrogen structures (at >200 GPa) arises from the intrinsic stability of its 6-member rings and has properties similar to carbon graphene.



Naumov I. I. and Hemley R. J. Aromaticity, Closed-Shell Effects and Metallization of Hydrogen, *Accts. Chem. Res.*, **47**, 3551 (2014).



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