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**Coronoid Nanographene C₂₁₆ as Hydrogen Purification Membrane: A
Density Functional Theory Study**

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Abstract: The first coronoid nanographene C₂₁₆ molecule, which is an extended polycyclic aromatic hydrocarbon containing a defined cavity, was studied throughly as a hydrogen purifier using the density functional theory and molecular dynamics simulations. It is demonstrated that C₂₁₆ is an effective ultimate membrane for hydrogen purification with a moderate penetrating energy barrier of about 0.615 eV. Furthermore, C₂₁₆ is superior to the porous graphene, polyphenylene, and other traditional membranes since the selectivity of H₂ to O₂, N₂, NO, H₂O, CO and CO₂ on C₂₁₆ surface is higher than other membranes. Meanwhile, the recent successful synthesis of nanographene C₂₁₆ in the laboratory provides the possibility of the industrial applications.

Keywords: Nanographene C₂₁₆, density functional theory, hydrogen purification membrane, selectivity, permeance.

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