Contribution ID: **229** Type: **Oral**

Helium separation of monolayer C_2N membrane under uniform strain

Thursday 25 May 2017 10:30 (15 minutes)

An efficient membrane for helium separation from natural gas is quite crucial for cryogenic industries. However, most experimentally available membranes fail in separating He from small molecules in natural gas, such as Ne, H_2, O_2, CO and N_2. Recently, a new 2D graphene-like sheet: C_2N was synthesized via a simple wet-logical reaction. C_2N has more advantage than among other porous 2D materials because it has large pore size of 5.52 Å. In this work, we calculated the energy barrier of gas molecules (Ne, H_2, O_2, CO, N_2) passing through the porous C_2N membrane by using first-principles calculations. The energy barrier of He, Ne, H_2, O_2, CO and N_2 are 0.029 eV, 0.070 eV, 0.067 eV, 0.128 eV, 5.817 eV and 0.070 eV, respectively. We found that energy barrier of He molecules is lowest among other gas molecules. This means C_2N can possibly separate He gas from natural gas. To reveal efficiency of membrane, the selectivity of He over Ne, H_2, O_2, CO, N_2 molecule has been calculated. The selectivity of He over Ne, H_2, O_2, CO, N_2 molecules respectively are 92.9, 32.4, 547, 1.46x10^7, and 4.37x10^9, respectively. Although energy barrier of He is lowest, selectivity clearly states that the C_2N membrane is not powerfully separate He gas from natural gas, especially from H_2 and Ne molecule. Moreover, we study the effect of applied uniform strain to the energy barrier and selectivity of membrane. We found that the energy barrier and the selectivity of gas molecule are exponentially lower as function of strain.

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Session Classification: A6: Condensed Matter and Accelerators

Track Classification: Condensed Matter Physics