Cover Picture

Yves Rubin, Thibaut Jarrosson, Guan-Wu Wang, Michael D. Bartberger, K. N. Houk, Georg Schick, Martin Saunders, and R. James Cross

The cover picture shows the process of hydrogen and helium insertion/expulsion which has been achieved for the first time with an open fullerene derivative (outlined in the background). The experimental activation barrier for helium decomplexation could be obtained and fully agrees with the calculated value (density functional theory). The barrier for H_2 complexation/decomplexation is interestingly almost double that of helium, as illustrated by the energy diagram shown in the foreground. This difference arises from the larger, elongated surface of H_2 undergoing greater van der Waals interaction at the transition state relative to that of helium, even though both atoms have the same radii. More about this process can be found in the article by Rubin, Houk, Saunders, Cross et al. on p. 1543 ff.