Pore mouth model	Radius Å	minimum
(5,5)	3.35	-1325.05
(6,6)	4.00	-937.31
(8,8)	5.38	-624.16

Table 6: Radii and global minimum potential energies in cm<sup>-1</sup> for different sizes of armchair pore mouth models. 2 unit translational cells have been used.



Figure 16: Ratio of rates  $(k_{D2}/k_{H2})$  for different armchair pore model structures with different radii versus temperature in Kelvin.

Nano tube	Radius Å	PF for 70K	PF for 150K	PF for 300K
(8,0)	3.14	5.65x10 <sup>6</sup>	$5.21 \times 10^3$	$4.92 \times 10^2$
(9,0)	3.43	3.55x10 <sup>6</sup>	6.12x10 <sup>3</sup>	$8.04 \times 10^2$
(10,0)	3.94	3.95x10 <sup>5</sup>	$4.03 \times 10^3$	$1.04 \times 10^3$
(11,0)	4.21	7.45x10 <sup>4</sup>	$2.42 \times 10^3$	$9.94 \times 10^2$
(12,0)	4.7	$3.42 \times 10^4$	$1.92 \times 10^3$	$1.00 \times 10^3$
(13,0)	5.02	1.63x10 <sup>4</sup>	$1.42 \mathrm{x} 10^3$	8.75x10 <sup>2</sup>

Table 7: Partition function for differently sized nanotubes employing the NW potential.



Figure 17: Minimum energy path for test structure employing the FB and the NW potentials.

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