

Toward In-Silico Modeling of Palladium- Hydrogen-Carbon Nanohorn Nanocomposites

*Piotr Kowalczyk^{*1}, Artur P. Terzyk², Piotr A. Gauden², Sylwester
Furmaniak² and Katsumi Kaneko³*

[1] Nanochemistry Research Institute, Department of Chemistry, Curtin
University of Technology, P.O. Box U1987, Perth, 6845 Western
Australia, Australia

[2] Department of Chemistry, Physicochemistry of Carbon Materials
Research Group, N. Copernicus University, Gagarin St. 7, 87-100 Torun,
Poland

[3] Center for Energy and Environmental Science, Shinshu University,
4-17-1 Wakasato, Nagano 380-8553, Japan

Corresponding author footnote (*To whom correspondence should be addressed):

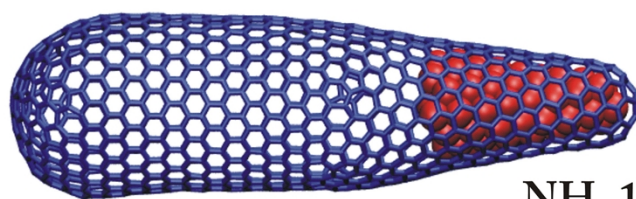
Dr Piotr Kowalczyk

Tel: +61 8 9266 7800

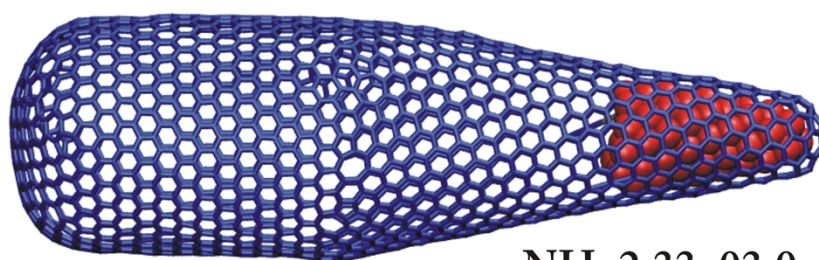
E-mail: Piotr.Kowalczyk@curtin.edu.au

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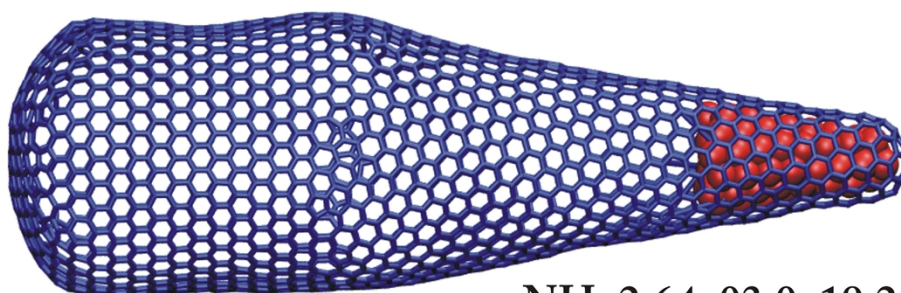
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NH_1.71_03.0_19.2



NH_2.33_03.0_19.2



NH_2.64_03.0_19.2

Figure 1S. Snapshots of Pd₈₁-SWCNH nanocomposites (top to the bottom: NH_1.71_03.0_19.2, NH_2.33_03.0_19.2 and NH_2.64_03.0_19.2 nanohorn¹) collected from temperature-quenched Monte Carlo simulations. Red spheres present the most stable morphologies of Pd₈₁ clusters confined in SWCNHs.

References

(1) S. Furmaniak, A. P. Terzyk, K. Kaneko, P. A. Gauden, Kowalczyk P., T. Itoh, The first atomistic modelling-aided reproduction of morphologically defective single-walled carbon nanohorns, *Phys. Chem. Chem. Phys.*, 2013, **15**, 1232-1240.