136a Computational Understanding of Growth Mechanism and Novel Properties of Silicon Nanowires [Invited]

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The shrinkage of dimensions of nanomaterials is expected to lead to fascinating properties related to size effects, which may be exploited for future exciting applications (e.g. optoelectronic, chemical and biological sensing). Different aspects of nanoscience and technology (nanomaterials structure, growth mechanisms and properties) can be studied by modern computational methods, providing insight where experimental methods cannot and predicting properties to guide experimentalists. Here, we present examples of computations that address different aspects of science and technology of silicon nanowires. These examples include: the mechanism of oxide-assisted formation of silicon nanowires [1]; the thin stable short silicon nanowires [2]; size-dependent oxidation of silicon nanostructures [3]; the possible silica nano-architectures including nanowires or nanorods, fully coordinated nanotubes, discrete fullerene-like cage, and porous zeolite-like 3D networks [4]; and results of energetic, chemical, electronic, optical and transport properties of nanostructured materials towards designs of nanoelectronics and nanosensors [5].

[1] Phys. Rev. Lett. 93, 095503 (2004); Adv. Mat. 15, 635 (2003); Phys. Rev. B64, 113304 (2001); J. Phys. Chem. B105, 1705 (2001); J. Chem. Phys. 114, 5531 (2001). [2] Phys. Rev. B65, 125305 (2002). [3] Appl. Phys. Lett. 88, 4223 (2002); J. Phys. Chem. B108, 1967 (2004). [4] Phys. Rev. B70, 205404 (2004); Phys. Rev. B69, 153403(2004); J. Phys. Chem. B108, 18451 (2004); Chem. Phys. Lett. 394, 437 (2004). [5] (a) Energetics and electronic: Phys. Rev. B65, 245417 (2002); J. Appl. Phys. 92, 7453 (2002); Chem. Phys. Lett. 364, 251 (2002). (2) Chemical: J. Chem. Phys. in press (2005); Chem. Phys. Lett. 398, 62 (2004). (3) Optical: J. Appl. Phys. in press (2005); Phys. Rev. B69, 115417 (2004). (4) Transport: J. Phys. Chem. B108, 16636 (2004); J. Appl. Phys. 95, 5729 (2004); Phys. Rev. B66, 045404 (2002).