$$\omega_{\text{Òi}}^2 = 80\,\text{B}^2\,\frac{\text{V}_0}{\text{e}^2\text{m}}\,\frac{\varepsilon_0(\varepsilon_1-1)}{\left(\frac{1}{2}\text{x}_\text{g}-\text{x}_\text{m}\right)^{12}}, \qquad (\omega'_{\text{Òi}})^2 = 80\,\text{B}^2\,\frac{\text{V}_0}{\text{e}^2\text{m}}\,\frac{\varepsilon_0(\varepsilon_2-1)}{\left(\frac{1}{2}\text{x}_\text{g}+\text{x}_\text{m}\right)^{12}},$$

где V_0 - классической объем электрона. Подставляя численных значений параметров, получаем, что

$$\omega_{\text{Òi}}^2 = 11\times10^{16}\,(\text{рад/с})^2,\ \ (\omega'_{\text{Òi}})^2 = 3.1\times10^{16}\,(\text{рад/с})^2.$$

В случае, когда на электрон действует как кулоновские, так и томас-фермиевские потенциалы, с учетом индукционных сил поля определим полную энергию колебательных систем, которая согласуется результатом эксперимента, а именно ЭДС меняет знак при частоте ω_0.

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EFFECT OF SURFACE PASSIVATION WITH DIFFERENT FUNCTIONAL GROUPS ON STABILITY OF SILICON NANOPARTICLES: QUANTUM CHEMICAL SIMULATION

Mukhtarov A.P., Normurodov A.B., Makhkamov Sh., Swihart M.T.
Institute of Nuclear Physics AS RUz, Ulughbek, Tashkent, ofm@inp.uz

Luminescence on silicon nanoparticles is very important effect due to their potential use as light emitters in displays or general illumination and as fluorescent probes for bioimaging. Si particles ranging from 1 to 5 nm in diameter exhibited photoluminescence (PL). However, the origin and characteristics of the luminescence are associated not only with the nanoparticle size but also with its shape and the nature of its surface.

The diamond-like structure of core Si atoms in small clusters can by stabilized only by termination of the dangling bonds of the surface Si atoms. The smallest (1 nm in diameter) model of blue-emitting Si particles with a diamond-like structure is an H-terminated, reconstructed Si_{24} cluster cage with one silicon tetrahedron in the interior ($Si_5Si_{24}H_{24}$). But H-terminated clusters are rather unstable in air and will be oxidized. The presence of O at the particle surface can introduce states within the band gap that lead to red-shifted emission. An effective means of stabilizing the silicon surface and PL properties is to graft an organic monolayer onto the H-terminated surface through a hydrosilylation reaction. These particles are quite resistant to oxidation.

Here the non-conventional tight-binding (NTB) method proposed by Khakimov[1] has been used for studying clusters with 29 silicon atoms. Geometries of fully and partially passivated nanoparticles have been fully optimized, without symmetry constraints, by a computational approach combining the above method with molecular dynamics (MD).

We studied the surface-dimerized Si_{29} cluster, with unbonded orbitals saturated by hydrogen atoms and hydrocarbon or hydroxyl groups. In particular, one, two, four and all hydrogen atoms of the $Si_{29}H_{24}$ cluster were substituted by CH_3 or OH groups. Only the C-Si, C-H and O-Si, O-H bonds and associated bond angles were optimized, while the remainder of the cluster was treated as a rigid body. The diameter of the $Si_{29}H_{24}$ nanocluster is ~1.1 nm. The cluster core of silicon atoms has 0.78 nm diameter.

On methylation of the $Si_{29}H_{24}$ cluster, the HOMO-LUMO gap narrowed up to 0.81 eV. That's less on 0.17 eV than for pure $Si_{29}H_{24}$ cluster (0.98 eV). Atom-atom repulsive energy, which includes electrons correlation effects is decreased by ~10% upon methylation. The covalent binding energy between silicon atoms is also diminished. That is probably caused by partial outflow of the electron density to the peripheral silicon atoms which are bonded with hydrogen. The charge on silicon atoms neighboring the methyl group remained the same as for the hydrogenated cluster. However, additional flow of electron density from the cluster to

carbon atoms is observed, leading to charge depletion at the core of the cluster. We have also calculated vertical and adiabatic ionization potentials of this system. Particular, the difference between vertical and adiabatic ionization potentials, when considering relaxation only of the methyl groups, was found to be 0.07 eV. The charge state of the cluster did not affect the repulsive force between the central silicon atoms. The charge induced into the cluster is basically allocated on peripheral silicon atoms while the charge on the central atom was kept constant. The clusters covered by hydrogen atoms were also indifferent to the cluster charge variations. Detachment of an electron from the cluster decreased the negative charge on the carbon atoms. Increasing the number of methyl groups on the cluster led to narrowing of the HOMO-LUMO gap. For the fully methylated Si_{29} cluster ($Si_{29}(CH_3)_{24}$), the double positive charged state was found to be most preferable. The diameter of the Si_{29} cluster covered fully by methyl groups was ~1.35 nm.

Calculations of the pure and hydrogenated Si_{29} cluster with one and two hydroxyl group on the surface were also performed. The neutral Si_{29} cluster with one –OH group was found to be less energetic favorable (by 2.89 eV) than bare Si_{29}, but was the most stable among the charged clusters with the same structure. Its vertical ionization potential was 11.2 eV. Its electron affinity was -0.58 eV. Adding one more (OH) onto this cluster increased the electron affinity up to -2.68 eV, while lowering its ionization potential to 2.23 eV. These clusters with a few hydroxyl groups were less stable than the parent $Si_{29}H_{24}$ cluster, at least when considering only Si-O-H bond relaxation. The cohesion energy of the $Si_{29}H_{23}$-OH cluster was -183.7 eV. Substituting one more hydrogen atom on the surface with a hydroxyl group led decreased the cohesion energy by 0.43 eV.

We also considered clusters with oxygen atoms bonded to one or two silicon atoms of the cluster surface. Oxygen bonded to one Si of the bare cluster made the negatively charged cluster more stable (by 3.17 eV) than the neutral one. The same oxygen bonded to the hydrogenated $Si_{29}H_{24}$ made the neutral cluster more favorable than other charge states. The vertical ionization potential for this cluster was 13.9 eV. The oxidation of H-terminated nanoparticles upon heating or under 254 nm UV radiation in Swihart's experiment[2-4], and the stability of the hydrocarbon covered particles, can be easily explained by breaking surface Si-H bonds, which requires ~3.75 eV, initiating subsequent oxidation. The Si-CH_3 binding energy is ~5.5 eV and therefore these bonds are stable against UV irradiation or moderate heating.

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ИЗУЧЕНИЕ ЗАКОНОМЕРНОСТЕЙ ДИФФУЗИИ И ВЛИЯНИЕ РЕДКОЗЕМЕЛЬНЫХ ЭЛЕМЕНТОВ НА ФИЗИЧЕСКИЕ ЭФФЕКТЫ В КРЕМНИИ

Назыров Д.Э.
Национальный университет Узбекистана имени Мирзо Улугбека, Ташкент
e-mail: dnazirov2004@mail.ru

В последние годы, кремний легированный редкоземельными элементами (РЗЭ), привлекает все большее внимание научных исследователей и технологов как перспективный материал для нано- и оптоэлектроники. Эффективность же примесей РЗЭ в кремнии, проявление их уникальных свойств в электронных структурах зависит как от спектра электрически и оптически активных центров, содержащих РЗЭ, так и общей концентрации, а также механизма диффузии РЗЭ в кремниевой матрице [1-5].

Основными задачами настоящего исследования являлись следующие: исследование закономерностей диффузии, растворимости, электрических свойств РЗЭ в монокристаллическом кремнии и их взаимодействия с примесями быстродиффундирующих и часто неконтролируемых примесных элементов, с термо- (ТД) и радиационными дефектами (РД), а также свойств *p-n*, МДП и МСП структур на основе кремния, легированного РЗЭ.

Проведены комплексные исследования закономерностей диффузии и растворимости примесей