Reverse Quantum Confinement-Strain Coupling in Ultra-Small Quantum Dots

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Abstract: In the present work we report on the investigation of ***reverse quantum confinement – strain coupling*** in quantum dots. While tremendous efforts have been expended to understand the impact of ***mechanical strain on the electronic band structures*** of quantum dots (and hence their opto-electronic properties) initial results of the author, based on both *ab initio* computations as well as simple analytical models, also suggest a startling ***reverse effect*** i.e. despite ***absence*** of external strains, if the quantum dot is made small enough (1-5 nm range), the band structure change due to quantum confinement may ***induce a strain*** in the quantum dot which in turn will alter the band structure and the latter in turn, will further alter the strain thus resulting in a nonlinear self-consistent type coupling. For simple particle-in-a-box type idealizations, in striking analogy to Bose-Einstein condensates, a nonlinear cubic Schrödinger's equation is found to be applicable. "Reverse coupling" provides another basis for novel size effects[1] in the band gaps of quantum dots beyond what is currently understood. Apart from a systematic investigation of this phenomena via the use of parameter-free *ab initio* methods (self-consistent density functional theory) we present coarse-grained multi-band envelope function based approaches to capture the essential features of the reverse coupling effect.

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[1] Other causes of size-effects (apart from the usual quantum confinement) are due to the size-dependency of mechanical strain at the nanoscale that is usually ignored in most works.