One-dimensional (1D) electronic systems are currently intensively investigated for both fundamental and technological reasons. With respect to future nanoelectronic device concepts the present work aims at generating a solid knowledge and detailed understanding about the physical foundations of such perspective future devices. Highly anisotropic surface superstructures have attracted considerable attention in this context. An acutely studied model system of this kind is the ordered atomic-scale array of self-assembled In nanowires that forms the Si(111)-(4×1)In phase at room temperature (RT) [1]. More than 10 years ago it was discovered that this nanowire array undergoes a reversible phase transition from (4×1)!(8×2) translational symmetry at T_C = 120 K [2]. However, while being discussed intensively in the scientific literature, both the (4×1)!(8×2) phase transition's driving mechanism and low temperature (LT) ground-state with its associated properties remain strongly controversial. In the present work the In/Si(111)-(4×1)/(8×2) nanowire array is investigated by means of state-of-the-art ab initio computer simulations. It is demonstrated that the longstanding problem of determining the internal structure and exact electronic properties of the nanowire array's LT ground-state cannot be resolved by the surface energetics alone. It turns out that the density functional theory (DFT) total-energy results for the In/Si(111)-(4×1)/(8×2) surface are extremely sensitive with respect to the details of the electron-electron interaction treatment. Electronic structure and transport calculations performed for the trimer and hexagon models of the LT ground-state indicate hexagon formation, as first suggested by González et al. [3]. These results demonstrate the distinct influence of small changes of the nanowire geometry on its conductance (cf. Publ. [11,12]). Given the ambiguities of the total-energy calculations in determining the internal structure of the (8×2) ground-state, the comparison of optical fingerprints calculated for structural candidates with measured data is expected to be helpful. Calculations of the anisotropic optical response in the visible and mid-infrared regime including intraband transitions have been performed for the In/Si(111)-(4×1)/(8×2) nanowire array for the first time. It is demonstrated that states close to the Fermi energy lead to distinct and unique optical fingerprints in the mid-infrared regime for each of the examined structural models. Only the spectra of the (8×2) hexagon model agree closely with recent measurements. These results are suitable to effectively conclude the search that has been ongoing for more than 10 years (cf. Publ. [1,6,7]). To address the driving mechanism of the phase transition the In/Si(111)-(4×1)/(8×2) surface's thermal properties have been explored by large-scale frozen phonon and molecular dynamics (MD) simulations. The results indicate that the soft shear mode mechanism, as proposed by González et al. [3], is at least partially correct. Two further soft phonon modes in conjunction with the shear mode facilitate the phase transition. By comparing the present results to the Raman spectroscopy measurements by Fleischer et al. [4] the existence of these soft modes could be confirmed for the first time. One-dimensional (1D) electronic systems are currently intensively investigated for both fundamental and technological reasons. With respect to future nanoelectronic device concepts the present work aims at generating a solid knowledge and detailed understanding about the physical foundations of such perspective future devices. Highly anisotropic surface superstructures have attracted considerable attention in this context. An acutely studied model system of this kind is the ordered atomic-scale array of self-assembled In nanowires that forms the Si(111)-(4×1)In phase at room temperature (RT) [1]. More than 10 years ago it was discovered that this nanowire array undergoes a reversible phase transition from (4×1)!(8×2) translational symmetry at T_C = 120 K [2]. However, while being discussed intensively in the scientific literature, both the (4×1)!(8×2) phase transition's driving mechanism and low temperature (LT) ground-state with its associated properties remain strongly controversial. In the present work the In/Si(111)-(4×1)/(8×2) nanowire array is investigated by means of state-of-the-art ab initio computer simulations. It is demonstrated that the longstanding problem of determining the internal structure and exact electronic properties of the nanowire array's LT ground-state cannot be resolved by the surface energetics alone. It turns out that the density functional theory (DFT) total-energy results for the In/Si(111)-(4×1)/(8×2) surface are extremely sensitive with respect to the details of the electron-electron interaction treatment. Electronic structure and transport calculations performed for the trimer and hexagon models of the LT ground-state indicate hexagon formation, as first suggested by González et al. [3]. These results demonstrate the distinct influence of small changes of the nanowire geometry on its conductance (cf. Publ. [11,12]). Given the ambiguities of the total-energy calculations in determining the internal structure of the (8×2) ground-state, the comparison of optical fingerprints calculated for structural candidates with measured data is expected to be helpful. Calculations of the anisotropic optical response in the visible and mid-infrared regime including intraband transitions have been performed for the In/Si(111)-(4×1)/(8×2) nanowire array for the first time. It is demonstrated that states close to the Fermi energy lead to distinct and unique optical fingerprints in the mid-infrared regime for each of the examined structural models. Only the spectra of the (8×2) hexagon model agree closely with recent measurements. These results are suitable to effectively conclude the search that has been ongoing for more than 10 years (cf. Publ. [1,6,7]). To address the driving mechanism of the phase transition the In/Si(111)-(4×1)/(8×2) surface's thermal properties have been explored by large-scale frozen phonon and molecular dynamics (MD) simulations. The results indicate that the soft shear mode mechanism, as proposed by González et al. [3], is at least partially correct. Two further soft phonon modes in conjunction with the shear mode facilitate the phase transition. By comparing the present results to the Raman spectroscopy measurements by Fleischer et al. [4] the existence of these soft modes could be confirmed for the first time.

(8×2) hexagon model agree closely with recent measurements. These results are suitable to effectively conclude the search that has been ongoing for more than 10 years (cf. Publ. [1,6,7]). To address the driving mechanism of the phase transition the In/Si(111)-(4×1)/(8×2) surface's thermal properties have been explored by large-scale frozen phonon and molecular dynamics (MD) simulations. The results indicate that the soft shear mode mechanism, as proposed by González et al. [3], is at least partially correct. Two further soft phonon modes in conjunction with the shear mode facilitate the phase transition. By comparing the present results to the Raman spectroscopy measurements by Fleischer et al. [4] the existence of these soft modes could be confirmed for the first time. In transport physics calculations and measurements are usually carried out at low bias, low temperature since the main focus is centered on fundamental principles. However, with respect to device applications the high temperature properties are most important. Based on the (8×2) hexagon model for the LT ground-state a combined frozen phonon and MD approach is presented to derive the temperature dependent transport properties including the phase transition. However, the classical energy distribution employed by MD calculations effectively prohibits a sufficiently accurate treatment of the highly subtle energetics of the In/Si(111)-(4×1)/(8×2) nanowire array. Instead a quantum Monte Carlo approach is proposed that incorporates both the correct potential energy landscape and energy distribution. As doping represents the basic building block of today's microelectronics first principles calculations of the Landauer conductance of doped In nanowires have been performed for various adatom species. Distinct conductance modifications are predicted that are related to potential well scattering, nanowire deformation or a combination of both effects. (cf. Publ. [4,9]).