Abstract Submitted
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Semiclassical potential functionals for semiconductor quantum wells ATTILA CANGI, Max Planck Institute of Microstructure Physics — Parabolic semiconductor quantum wells are considered promising candidates for constructing devices emitting radiation in the largely unexplored THz regime. However, progress is impeded by the difficulty of fine-tuning intersubband transitions in these quantum wells which is achieved by modifying the quantum-well geometry and mixing different materials. We predict the electronic structure of parabolic semiconductor quantum wells highly efficiently by iterating the Kohn-Sham self-consistent cycle without solving the Kohn-Sham equations[1]. We achieve this by combining potential functionals[2,3] with a recently derived semiclassical approximation[4]. This (1) demonstrates our method's efficiency and accuracy for realistic systems and (2) illustrates its utility as a high-throughput method for predicting the electronic structure of technologically intriguing microstructures. [1] A. Cangi, C.R. Proetto, S. Pittalis, K. Burke, and E.K.U. Gross, submitted (2016). [2] A. Cangi, D. Lee, P. Elliott, K. Burke, and E.K.U. Gross, PRL 106, 236404 (2011). [3] A. Cangi, E. K. U. Gross, and K. Burke, PRA 88, 062505 (2013). [4] R.F. Ribeiro, D. Lee, A. Cangi, P. Elliott, and K. Burke, PRL 114, 050401 (2015).

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