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Spontaneous charge carrier localization in extended one-dimensional systems VOJTĚCH VLČEK[1], HELEN EISENBERG, Hebrew University of Jerusalem, Israel , GERD STEINLE-NEUMANN, Bayerisches Geoinstitut, Universität Bayreuth, Germany, ROI BAER, Hebrew University of Jerusalem, Israel — Charge carrier localization in extended atomic systems can be driven by disorder, point defects or distortions of the ionic lattice. Herein we give first-principles theoretical computational evidence that it can also appear as a purely electronic effect in otherwise perfectly ordered periodic structures and we show that electronic eigenstates can spontaneously localize upon excitation. Optimally-tuned range separated density functional calculations reveal that in trans-polyacetylene and polythiophene the hole density localizes on a length scale of several nanometers. This is due to exchange induced translational symmetry breaking of the charge density. Ionization potentials, optical absorption peaks, excitonic binding energies and the optimally-tuned range parameter itself all become independent of polymer length when it exceeds the critical localization length scale. These first-principles findings show, for the first time, that charge localization is not caused by lattice distortion but rather it is their cause, changing the physical models of polaron formation and dynamics, helping to explain experimental findings that polarons in conjugated polymers form instantaneously after exposure to ultrafast light pulses.

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