

One-hundred-nanometer-scale electronic state and transport calculations of organic device material on the K computer

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The 100-nanometer-scale electronic-state and transport calculations were carried out for flexible (organic) devices or key devices of Internet of Things (IoT) [1,2] (Fig. 1). Our original massively-parallel electronic structure calculation code ELSSES (<http://www.elses.jp>) shows a high parallel efficiency, the strong scaling, with 10^8 atoms up to the full node calculations of the K computer. The method is an order- N calculation and uses a modelled (transferable TB) theory based on *ab initio* calculations. Recently, the method also realises quantum transport calculation by wavepacket dynamics method, in which an effective Schrodinger-type equation ($i\partial_t\psi = H\psi$) is solved for hole or electron wavepacket ($\psi = \psi(\mathbf{r}, t)$). A crucial role in transport is played by ‘semi-localized’ π wavefunctions that spread over several monomer units. The difference in mobility among various structures of an organic polymer (poly-(phenylene-ethynylene, PPE)[3] were reproduced [1]. An analysis on 10^8 -atom condensed PPE’s presents a transport mechanism through the dynamical small polymer networks [2]. A future outlook is the combined research among simulation and data scientific analysis and a preliminary work appears in the poster session [4]. Acknowledgement: We thanks T. Tada (Tokyo Tech.) and M. Ishida (Sumitomo Chemical Co. Ltd.) for collaborations.

[1] H. Imachi, et al., in press; <http://arxiv.org/abs/1603.09616>

[2] T. Hoshi et al., in press; <http://arxiv.org/abs/1609.08377>

[3] J. Terao, et al, Nature Comm. 4, 1691 (2013)

[4] H. Imachi, et al, poster in this workshop.

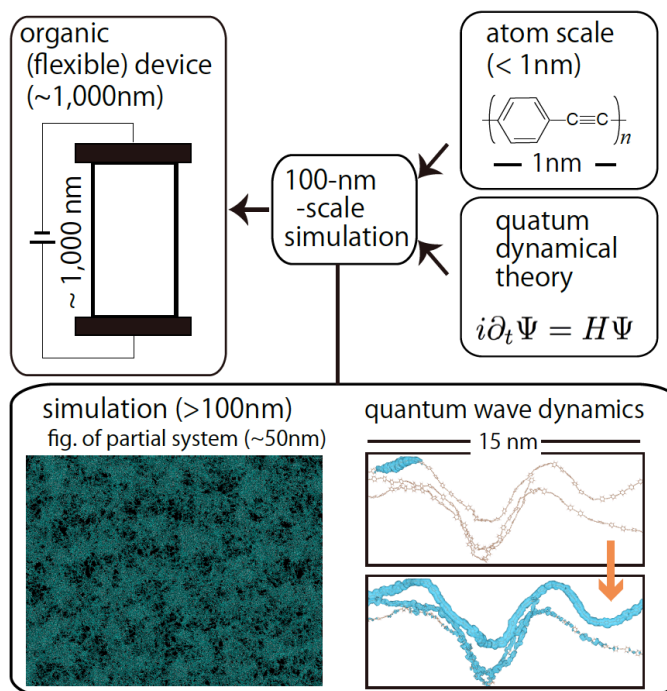


Fig. 1 (right) The overview of the present work with 100-nm-scale or 10^8 atoms electronic state calculations (lower left) and quantum wavepacket dynamics (lower right).