Theoretical Design of Materials with Innovative Functions Based on Element Strategy and Relativistic Electronic Theory

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Theoretical material design requires a theory with chemical accuracy. Most of rare or restricted elements are heavy elements, of which relativistic effects cannot be neglected. However, most of quantum chemical calculations are currently performed by means of the non-relativistic treatment based on the Schrödinger equation, where the relativistic effect is considered in an ad-hoc manner. Such situation renders theoretical design in chemical accuracy difficult.

The purpose of this study is to establish a practical relativistic quantum chemical theory based on the Dirac equation. On the basis of the relativistic theory, material design of has been conducted in terms of innovative catalytic activity, electromagnetic property, electronic functional material, photobiological function, and functional polymer.

In the former topic, a linear-scaling method for the two component relativistic theory was developed [1,2]. As shown in Fig. 1, our method (DC-LUT-IODK) is much faster than the conventional methods (4c, X2C, and IODK) and has similar computational cost to the non-relativistic calculation (DC-NR).

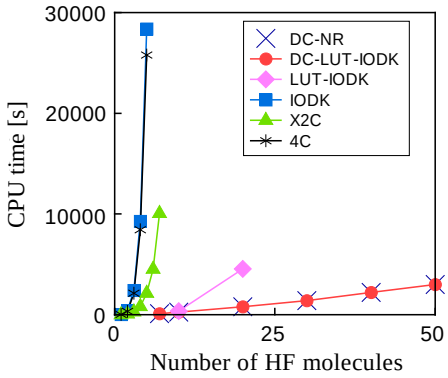

Fig. 1. Comparison of CPU time.

As for the design of functional materials, we will present theoretical design of materials for dye-sensitized solar cells and screening of substances for non-lead perovskite solar cells.

In addition, we have conducted joint researches. Here, the computational result of stable organic radicals is shown in Fig. 2. Large-scale calculations using our original method realized the reproduction of near-infrared photoabsorption [3].

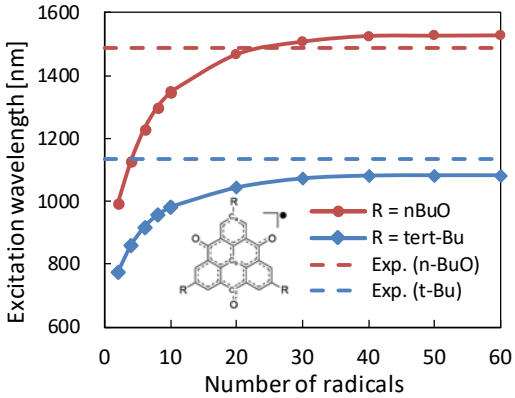

Fig. 2. Calculated absorption wavelengths of organic radical aggregates.

Bibliography

[1] J. Seino and H. Nakai; J. Chem. Phys., **139**, 034109 (2013).

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[3] Y. Ikabata, Q. Wang, T. Yoshikawa, A. Ueda, T. Murata, K. Kariyazono, M. Moriguchi, H. Okamoto, Y. Morita, H. Nakai; npj Quantum Materials, **2**, 27 (2017).

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