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**Quantum Simulation of Electronic Structure by Quantum Coupled-Cluster with a Trapped Ion System** SHEN YANGCHAO, XIANG ZHANG, SHUAINING ZHANG, JIN-NING ZHANG, MAN-HONG YUNG, KIH-WAN KIM, Center for Quantum Information, IIIS, Tsinghua University — We report an experimental simulation of the electronic structure of a molecular ion based on a quantum version of the coupled-cluster method. The quantum method combines essential features from both classical and quantum computation in a way that can go beyond the limitations of the classical implementation of the unitary coupled-cluster method. The implementation was performed using a trapped multi-level ion ( $^{171}\text{Yb}^+$ ) controlled by microwave. The energies of the ground and excited states of a Helium hydride ( $\text{HeH}^+$ ) were obtained as a function of the nuclear separation. The effects of a simulated electric field on the chemical bond beyond the perturbation regime were studied. Our results represent a step towards a new and practical approach for studying various molecular process through quantum simulation. This work was supported by the National Basic Research Program of China under Grants No. 2011CBA00300 (No. 2011CBA00301), the National Natural Science Foundation of China 11374178 and 041303016.

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