講演会

日時　１０月５日午後４時より
場所　総合情報センタ・視聴覚室

講演者	**Michael W. Schmidt 博士** （アイオア州立大学化学教室） （アイオア州立大学エイムズ研究所 Senior Researcher）
タイトル	**Parallelization of an electronic structure code**
要　旨	The strategy for parallelization of the GAMESS electronic structure code will be described. Such codes typically contain many different computational kernels, with data storage ranging from $O(N^2)$ to $O(N^4)$, and with computational costs of $O(N^3)$ to $O(N^7)$. The choices made reflect the nature of the constantly changing hardware, including the interconnection, and the available support software, in addition to the nature of the quantum chemistry calculation itself. Efforts to produce effective parallel code in GAMESS have been underway since 1993, when a parallel direct SCF program was introduced. Distributed memory programming was introduced in 1999 to support a parallel MP2 gradient code, through a library called the Distributed Data Interface. The latest enhancement of our DDI support software was introduced in 2004, to optimize distributed memory programming on the ubiquitous SMP nodes. The goal, of course, is to allow efficient, scalable computation of molecular wavefunctions, not only for large molecules, but also for more complex and accurate ansaetze. A summary of the present capabilities and performance data of GAMESS will be included.

講演者	松永　仁城太　准教授 (Matsunaga Nikita) （ニューヨーク州ロングアイランド大学）
タイトル	**Toward Single-Molecule Electronic Devices**
要　旨	Can we use a single molecule as a component of electronic device? This question comes out naturally in facing inevitability that the dimension of device component approaching molecular dimension, if we are to continue the progress according to Moore's Law. Among many candidate molecules, conjugated organic molecules are best suited for nanoelectronics. Conduction mechanisms of single molecule electronic devices are investigated.

注意．この講演会は，理学系研究科における平成 16 年度後期開講の量子化学の第 1 回講義 (10/7) とするので，受講予定者は出席しアンケートを提出すること．