Spin Manipulation at Surfaces

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We entered the 21st Century witnessing several remarkable developments in Science and Technology. Novel materials and devices that were once considered *science fiction* materials are now, one after the other, becoming a reality. On the other hand, as is always the case, progress comes at a price. In the process of the continuing progress in Science and Technology, we encounter new problems and phenomena where conventional techniques and routines no longer apply. In particular is the astonishing development seen in nanometer scale technology, a domain we now call as Nanotechnology. To meet the ever-increasing demand for better large scale integration, basic components of devices are getting smaller, with the size ranging from the nanometer-scale to atomic-scale level. With this, one can easily realize that *Quantum Effects* are becoming more important. (We are currently in the stage of discovering the significance of Quantum Effects in the field of Nanotechnology.) However, it is not an exaggeration if we say that with further development; there will come a time when the basic material entity that is now used to build a device would be developed to function as a device itself. Given these circumstances, there will be high demands and necessities in developing novel theoretical routines and techniques that could quickly and efficiently find novel materials for synthesis that would suit our objectives. These necessary theoretical routines and techniques should incorporate quantum mechanics *per se*, and should not be dependent on experimental results and/or empirical parameters. *Ab-Initio/First Principles Calculations* satisfy all these requirements.

With recent developments in computational techniques, coupled with the rapid progress in terms of efficiency and computational capability of present computers, ab-initio/first principles-based *COMPUTATIONAL MATERIAL DESIGN* (**CMD®**) [1] is now a reality. Its impact/influence on industrial R&D is becoming very significant and will increase in the successive years. It is worth mentioning that there are already several precedents of patents granted for application based purely on the application of CMD® techniques, and more are expected to follow.

At the meeting, we will briefly introduce some applications of CMD® for magnetism control, e.g., real space image of the Kondo effect and influence of the RKKY interaction [2-7], surface spintronics device (Patent No. US 7,432,573 B2) [8], and enhancing oxygen reduction reaction on spin-polarized metal surface for fuel cell applications [9-11].

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