

Report

Workshop title: Theoretical and Computational Modeling of Magnetically Ordered Molecules & Electronic Nano-Transport of Spins: State of Art and Unanswered Questions : “The Como Moments”.

Organized by: Carlo M. Canali (Nordforsk Network Lead, Sweden)

Principle Investigator for distribution of US BES Travel Support: Tunna Baruah

DOE grant number : DE-SC0010744

As a culmination of a five-year Nordforsk Network project entitled “Nanospintronics: Theory and Simulations”, Professor Carlo Canali (Linneaus University, Sweden) and members of the network, and Vincenza Benza (Local Organizer Milan) organized a summer workshop in conjunction with the A. Volta Scientific Cultural Exchange program. This workshop took place 24-30 August 2013. Several Basic Energy Scientists from the US conducted lectures and also provided hands-on tutorials to developing materials and chemicals scientists. We have received a total of \$10,000 of support to offset the travel expenses of US-based participants for this workshop.

Nearly fifteen senior participants that are experts in the area of molecular magnetism (theory and experiment), electron transport, theoretical condensed matter physics, quantum chemistry, data-enabled design of molecular photon absorbers, and many-body theory participated in the workshop. The workshop combined lectures as well as hands-on computational tutorials to address various aspects of the simulations. The funding received from BES helped in supporting the travel expenses of following US participants from various universities:

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| 1. Jianwei Sun, Temple University | : \$1587.70 |
| 2. Joshua Borycz, University of Minnesota | : \$2603.16 |
| 3. Alex McCaskey, Virginia Tech | : \$1680.20 |
| 4. Xiangguo Li, University of Florida | : \$1568.10 |

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| Total : | \$7439.16 |
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The above-mentioned US participants have attended the talks and tutorials presented in the workshop and further demonstrated their understanding through generation of data for a number of small molecular magnets.

The PI thanks the BES support, which enabled the young US based researchers to attend the COMO Moments workshop.

