Atomic Scale Simulations in Materials Science and Biochemistry

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The common denominator of this presentation is a general overview is the development, implementation and application of the most advanced computational tools in the field of first principles and hybrid QM/MM (quantum mechanics / molecular mechanics) dynamical simulations techniques. These represent nowadays a general tool to perform accurate virtual experiments able to complement and to extend the insight provided by actual experiments. Free energy sampling techniques can be efficiently coupled to these methods to simulate activated processes and to workout reaction pathways. The range of applications where these methodologies are exploited extends from solid state physics to surface chemistry and to biochemical reactions. We shall focus on selected examples, corresponding to projects done in collaboration with major Japanese universities and laboratories. More specifically, patterning of graphene-based materials [1] and enzymatic reactions for green chemistry [2,3] will be presented as representative examples of atomic-scale driven processes having a macroscopic impact in nanotechnology and life science.

[1] Koizumi K., Boero M., Shigeta Y., Oshiyama A., *J. Phys. Chem. Lett.* **4**, 1592 (2013)
[2] Kamiya K., Baba T., Boero M., Matsui T., Negoro S., Shigeta Y., J. Phys. Chem. Lett. **5**, 1210 (2014)
[3] Baba T., Boero M., Kamiya K., Ando H., Negoro S., Nakano M., Shigeta Y., Phys. Chem. Chem. Phys. **17**, 4492 (2015)

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Education
1994 PhD, Physics - University of Turin (Italy) and École Polytechnique Fédérale de Lausanne EPFL-IRRMA (Switzerland)

Professional Experience
1/1995~7/1995 - Post-Doc at EPFL-IRRMA (Switzerland)
8/1995~4/1996 - Post-Doc at IBM Zurich Research Laboratory (Switzerland)
5/1995~5/1998 - Post-Doc at Max-Planck-Institut, Stuttgart (Germany)
5/1998~3/2001 - Post-Doc. JRCAT-AIST, Tsukuba (Japan)
4/2001~8/2002 - NEDO Fellow at AIST-RICS, Tsukuba (Japan)
9/2002~12/2008 - Associate Professor at University of Tsukuba (Japan)
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Fields of Research
Molecular simulations and modeling in condensed matter and biosciences. Visiting Full Professor at University of Tokyo – Computational Materials Science Initiative (CMSI) Project member (Japan); Visiting Full Professor at European Center for Atomic and Molecular Calculation - CECAM (Switzerland). Scientific director of the HPC Meso-Center (Equipex EQUIP@MESO). Author of more than 130 publications, among which 112 original research papers, 7 review articles, 6 book chapters, and 22 proceedings of international conferences. Results of ISI-Web-of-Science of 27/03/2015: Number of citations: 3343, h-index: 31

Publications
(Selection of 5 relevant publications)

1. F. L. Gervasio, M. Boero and M. Parrinello, Angew. Chem. Int. Ed. **45**, 5606 (2006)
2. M, Boero, T. Ikeda, E. Ito and K. Terakura, J. Am. Chem. Soc. **128**, 16798 (2006)
3. B. W. Heinrich, L. Limot, C. Iacovita, M. V. Rastei, J.-P. Bucher, D. Mbongo Djimbi, C. Massobrio and M. Boero, Phys. Rev. Lett. **107**, 216801 (2011)
4. K. Koizumi, M. Boero, Y. Shigeta and A. Oshiyama, J. Phys. Chem. Lett. **4**, 1592 (2013)
5. K. Kamiya, T. Baba, M. Boero, T. Matsui, S. Negoro, Y. Shigeta, J. Phys. Chem. Lett. **5**, 1210 (2014)