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VABILO NA PREGLOV KOLOKVIJ / INVITATION TO THE PREGL COLLOQUIUM

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Četrtek / Thursday, 22. 08. 2013, ob / at 13:00

**Velika predavalnica Kemijskega inštituta / Lecture Hall at the
National Institute of Chemistry; Hajdrihova 19, Ljubljana**

Four Adventures in Quantum Chemistry

Abstract:

Although today's powerful computers allow computational chemists to generate data without much effort, it is easy to produce so many numbers that we lose sight of the really important questions. In quantum chemistry, as in many other areas of science, the most important advances come from new conceptual insights, not new numbers. It is therefore essential that we continue to seek deeper understanding. ("Give us insight, not numbers" -- Charles Coulson, 1960)

In this lecture, I will describe four topics to which my research group has recently contributed:

1. Exact solutions of the Schroedinger equation for simple model systems [1,2]
2. Posmom - a variable that probes both the position and the momentum of an electron [3,4]
3. MOM - a simple method for modelling electronic excited states [5,6]
4. Dual-basis methods for performing accurate calculations quickly [7,8]

The lecture will be accessible to chemists and physicists, from both experimental and theoretical backgrounds. It will not assume a high level of specialist knowledge.

- [1] PF Loos and PMW Gill, Phys Rev Lett 103 (2009) 123008
- [2] PF Loos and PMW Gill, Phys Rev Lett 108 (2012) 083002
- [3] YA Bernard and PMW Gill, New J Phys 11 (2009) 083015
- [4] YA Bernard and PMW Gill, J Phys Chem Lett 1 (2010) 1254
- [5] ATB Gilbert, NA Besley and PMW Gill, J Phys Chem A 112 (2008) 13164
- [6] NA Besley, ATB Gilbert and PMW Gill, J Chem Phys 130 (2009) 124308
- [7] J Deng, ATB Gilbert and PMW Gill, J Chem Phys 130 (2009) 231101
- [8] J Deng and PMW Gill, J Chem Phys 134 (2011) 081103

Vljudno vabljeni! / Kindly invited!

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