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Guest Editorial

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Guest Editorial



This issue of *Molecular Simulation* is dedicated to the memory of Dr José Antonio Mejías Romero, who passed away, after a valiant fight against cancer, on 17 July 2008. Most of the articles included in this Special Issue were written by friends and colleagues who worked and collaborated with him during his fruitful, although truncated, scientific career.

José Antonio was born in Huelva, Spain, on 29 May 1967. He received his education in Chemistry from the University of Seville, where he obtained his Bachelor's degree in Chemistry in 1991. In 1994, he presented his PhD in this university with a dissertation entitled 'Quantum-mechanical description of local phenomena in multi-electron systems: Adsorption processes and magnetism in ionic solids'. After finishing his PhD, he collaborated with the Institute of Materials Science of Seville. In 1996, he spent 6 months in the University of

Bochum, Germany, after which he joined the Department of Earth Sciences of the University of Oxford, where he stayed until 1998. In October 1998, he moved to the just recently founded University *Pablo de Olavide* of Seville (UPO), at the same time that the Faculty of Experimental Sciences started its history with the new studies of Environmental Sciences. In September 2002, he was appointed as Associate Professor in the Physical Chemistry Group of this University. In September 2008, he was awarded with the Honour Medal of the UPO as a posthumous recognition.

José Antonio was a noted member of the pioneer team of teachers and researchers that helped to launch the new experimental studies at the UPO and contributed to build and develop the research laboratories of the Physical Chemistry Group. He underwent from the very beginning the rewards and frustrations characteristic of any new scientific and academic project, and faced them with enthusiasm and self-determination. José Antonio started from scratch the new subjects of Physics, Chemistry and Atmospheric Pollution for Environmental Sciences studies at the UPO. He devised guides, teaching material and laboratory exercises that are still used by the members of the group. He was initially trained as a theoretical chemist, and he acquired a vast scientific knowledge of the theoretical methods used in the study of crystals, surfaces, gases, liquids and nanoparticles, involved in a wide range of fields, such as atmospheric chemistry, photocatalysis, nucleation, magnetism and surface chemistry. He gradually increased his scientific interests by collaborating with experimentalists, and eventually he set up a new experimental research group focused on the study of functionalised metallic and semiconductor nanoparticles with applications in environmental sciences (ultrasensitive detection of pollutants), biotechnology and nanomedicine (biological labelling by luminescent quantum dots, selective drug delivery). He left behind an active research group with two collaborators and two PhD students who are carrying on with the equipment, experimental set-up, funding and ideas that he decisively contributed to achieve.

It is impossible to finish up this Editorial without any remark about the charisma and human features of José Antonio. He was good-humoured, cheerful, witty, smart,

incredibly funny, shockingly frank, tenderly childish and immensely kind hearted. These qualities remained and even shone brighter when he knew of the disease he suffered from. Those who knew him will never forget the incredible determination and enthusiasm with which he carried on with his work and vital projects, the care and tenderness towards his family and the courage with which he faced the last stage of his life. To us he was a sort of an everyday hero, a source of inspiration for our careers and lives, an irreplaceable colleague and friend.

We thank all the participants who contributed to this Special Issue, with special gratitude to the Editor in Chief of Molecular Simulation, Professor Nicholas Quirke. We send our greetings to his widow Pilar, his parents Concha and Andrés and to his brother and sister Andrés and Sole. *Un fuerte abrazo para todos ellos.*

Juan Antonio Anta, Sofía Calero and Said Hamad
Seville, May 27th, 2009