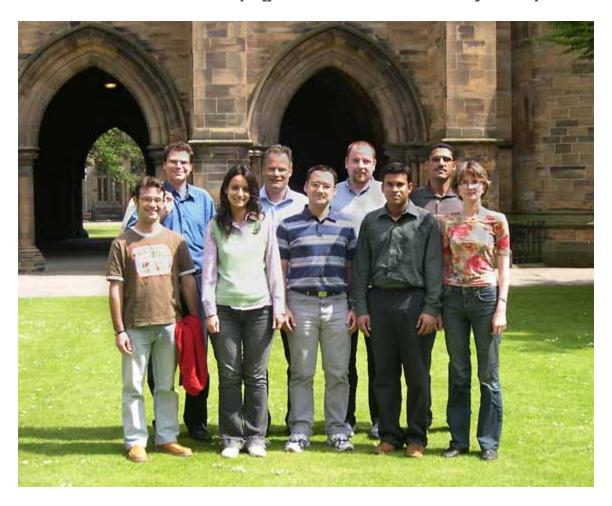


COMPUTATIONAL CHEMISTRY The McGrady group

Home | Members | Research | Publications | Resources | Links

Welcome to the webpages of the John McGrady Group!



The group's research interests focus on the electronic structure of inorganic systems in the broadest sense. We apply modern computational methods (typically density functional theory) to a diverse range of problems drawn from both transition-metal and main-group chemistry. The vast majority of our work involves close collaboration with experimental groups involved in the study of structure, spectroscopy, electrochemistry and reactivity.

You can find out more about our <u>research interests</u> and see a list of some recent <u>representative</u> <u>publications</u>.

PhD studentships available

Fully funded PhD positions are available on a variety of computational chemistry projects.

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