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Stefan Bromley (1971) is an ICREA Research Professor at the Institute of Theoretical and Computational Chemistry at the University of Barcelona (IQTC-UB) where he heads the Nanoclusters and Nanostructured Materials group. He obtained his PhD in Computational Physics (University of Southampton, UK) in 1997 and has held research posts in the UK (Postdoctoral fellow, Royal Institution), the Netherlands (Associate Professor, Delft University of Technology) and Spain (Ramón y Cajal fellow, UB). He has published ~150 WoS-listed articles and 8 book chapters, which have received over 4000 citations (h-index = 33), and has given many invited talks about his work at international conferences and academic institutions. He is also editor of a book on "Computational Modelling of Inorganic Nanomaterials".

## Research interests

With the constant technological drive for device miniaturisation, materials are increasingly being used at scales of only a few 100s or 1000s of atoms (i.e. the nanoscale). Such nanomaterials often display novel size-dependent properties compared to materials at everyday length scales. Using powerful supercomputers and both atomistic and quantum modelling methods, we aim to provide a detailed predictive understanding of the structural, electronic and chemical properties of nanomaterials. Our focus is on how nanomaterials evolve with increasing size, and designing new materials from nanoscale building blocks. Our research follows three main themes: (i) nanoclusters and nanostructured materials for energy applications (e.g $TiO_2$, ZnO), (ii) nucleation and properties of astronomically important nanomaterials (e.g. TiC, silicates), (iii) design of nanostructured materials using organic molecular building blocks for electronics/spintronics.

## Selected publications

– Ko KC, **Bromley ST**, Lee JY & Illas F 2017, 'Size-Dependent Level Alignment between Rutile and Anatase TiO2 Nanoparticles: Implications for Photocatalysis', *Journal Of Physical Chemistry Letters*, 8, 22, 5593 – 5598.
– Alcon I, Vines F, Moreira IPR & **Bromley ST** 2017, 'Existence of multi-radical and closed-shell semiconducting states in post-graphene organic Dirac materials', *Nature Communications*, 8, 1957.
– Alcon I, Reta D, Moreira IPR & **Bromley ST** 2017, 'Design of multi-functional 2D open-shell organic networks with mechanically controllable properties', *Chemical Science*, 8, 2, 1027 – 1039.
– Franco C, Mayorga Burrezo P, Lloveras V, Caballero R, Alcon I, **Bromley ST**, Mas-Torrent M, Langa F, Lopez Navarrete JT, Rovira C, Casado J, Veciana J 2017, 'Operative Mechanism of Hole-Assisted Negative Charge Motion in Ground States of Radical-Anion Molecular Wires', *Journal Of The American Chemical Society*, 139, 2, 686 – 692.
– Lamiel-Garcia O, Cuko A, Calatayud M, Illas F & **Bromley ST** 2017, 'Predicting size-dependent emergence of crystallinity in nanomaterials: titania nanoclusters versus nanocrystals', *Nanoscale*, 9, 3, 1049 – 1058.
– Kerkeni B, Bacchus-Montabonel M-C & **Bromley ST** 2017, 'How hydroxylation affects hydrogen adsorption and formation on nanosilicates', *Molecular Astrophysics*, 7, 1 – 8.
– Vines F, Lamiel-Garcia O, Illas F & **Bromley ST** 2017, 'Size dependent structural and polymorphic transitions in ZnO: from nanocluster to bulk', *Nanoscale*, 9, 28, 10067 – 10074.
– Mora-Fonz D, Lazauskas T, Woodley SM, **Bromley ST**, Catlow CRA & Sokol AA 2017, 'Development of Interatomic Potentials for Supported Nanoparticles: The Cu/ZnO Case', *Journal Of Physical Chemistry C*, 121, 31, 16831 – 16844.