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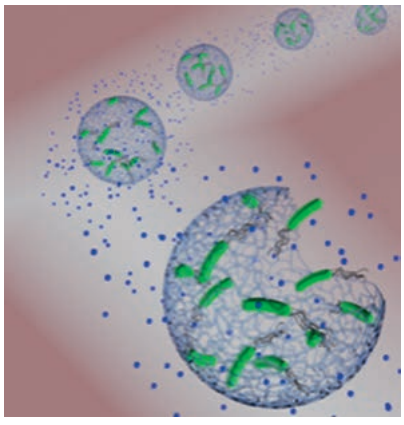
Short Abstracts of Interesting Recent Publications of Swiss Origin

Monodisperse selectively permeable hydrogel capsules made from single emulsions drops

Mathias Steinacher, Alice Cont, Huachuan Du, Alexandre Persat, Esther Amstad*, *ACS Appl. Mater. Interfaces* **2021,** 13, 15601–15609, https://dx.doi.org/10.1021/acsami.1c00230.
École Polytechnique Fédérale de Lausanne (EPFL)

Hydrogel capsules are used to entrap molecules with chemical or biological activity with a fine control of their release. However, their performance is dependent on the thickness and composition of the shells, often limiting their applications. In this work, the strategy to capsules with controlled dimensions using microfluidics has been brought to the next level, by developing a robust and scalable method to produce monodisperse microcapsules with thin hydrogel shells from single emulsion drop templates. This was achieved by selectively polymerizing acrylate-containing reagents near the drop surface. This strategy offers an additional benefit: it eases the functionalization of the capsules because acrylate-containing precursors possessing different functionalities can be easily incorporated into the shell, thereby, for example, allowing the design of capsules with an increased bioactivity. Moreover, the liquid core enables the growth of living microorganisms. The potential applications of this method encompass drug screening, observation of living species or the removal of waste products from water.

Authors' comments:
"This work introduces a fast, scalable approach to fabricate capsules composed of a thin size-selective hydrogel shell whose volume accounts for as little as 6% of the capsule volume."

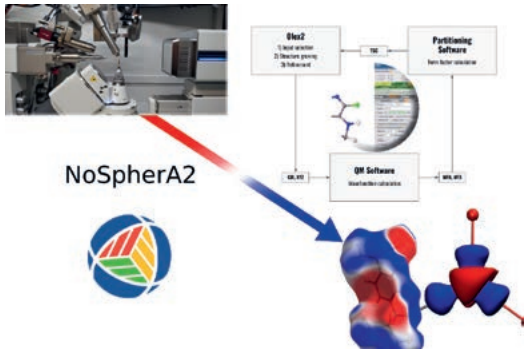


Accurate crystal structures and chemical properties from NoSpherA2

Florian Kleemiss[a], Oleg V. Dolomanov[a], Michael Bodensteiner[c], Norbert Peyerimhoff[d], Laura Midgley[d], Luc J. Bourhis[e], Alessandro Genoni[f], Lorraine A. Malaspina[a], Dylan Jayatilaka[g], John L. Spencer[h], Fraser White[i], Bernhard Grundkötter-Stock[j], Simon Steinhauer[j], Dieter Lentz[j], Horst Puschmann[b]*, and Simon Grabowsky[a]*, *Chem. Sci.* **2021**, *12*, 1675, https://doi.org/10.1039/d0sc05526c.
[a]Universität Bern, Switzerland; [b]OlexSys Ltd, UK; [c]Universität Regensburg, Germany; [d]Durham University, UK; [e]Bruker France, France; [f]Université de Lorraine & CNRS, France; [g]University of Western Australia, Australia; [h]Victoria University of Wellington, New Zealand; [i]Rigaku Europe SE, Germany; [j]Freie Universität Berlin, Germany

The relationship between a molecule's physicochemical properties and its structure is one of the key concepts of chemistry. For this, structural data has rocketed since the 1970s, when diffraction equipment became widely available. Most of the techniques used for the refinement of the structure, though, are still relying on over-simplifications to make up for the limited computing power available at the time. One of the main simplifications was the use of the Independent Atom Model, which assumes all atoms are separate, non-interacting spherical entities. Nonetheless, computational chemistry has evolved massively in the last years, providing much more potent and robust tools, such as software for quantum chemical calculations. NoSpherA2 (Non-Spherical Atoms in Olex2) takes advantage of such new tools, to provide a fast, reliable, and up to date software for the refinement of chemical crystal structures using the non-spherical structure refinement (Hirshfeld atom refinement) within Olex2.

Authors' comments:
"Huge investments in large-scale facilities for structural science (such as synchrotrons, free electron lasers, spallation sources) are taken around the world, but the analysis software tools are lagging behind. We combine modern data with modern methods to improve chemical interpretation of structure."



Prepared by Ana I. Benítez-Mateos, David Roura Padrosa, Gordon Honeyman, Keir Penston, and Francesca Paradisi*
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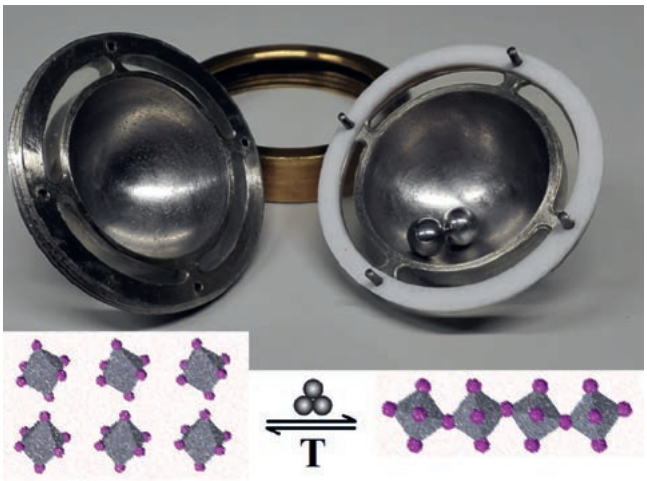
Metastability and Seeding Effects in the Mechanochemical Hybrid Lead(II) Iodide Formation

M. Wilke, D. J. Gawryluk, and N. Casati* *Chem. Eur. J.,* **2021**, 27, 5944–5955, https://doi.org/10.1002/chem202004431.
Paul Scherrer Institute

The mechanochemical synthesis of $(C(NH_2)_3)_3PbI_5$ (**X1**) and $(C(NH_2)_3)_4PbI_6$ (**X2**) was investigated. Using different mixing speed and energies whilst probing the reaction *via in situ* powder X-ray diffraction, their formation and interconversion was scrutinized. Dividing the overall reaction into single parts, it was proved that the formation of **X1** is dependent on the energy and mixing speed deployed. The nucleation of **X2**, however, is slightly negatively dependent on energy, but it is wholly dependent on mixing speed. Growth is broadly independent of other factors. Formation of **X2** is likely to be an auto-catalytic process, whereas **X1** is metastable. It can be stabilized by energy, which alongside mechanochemistry, can also be achieved by temperature. Results showcase the complexity of mechanochemical reactions.

Authors' comments:
«Mechanochemistry, reacting solid chemicals without solvents, is in its infancy. While its usage keeps expanding, the parameters affecting the reaction mechanisms are still to be fully understood.»



On-Surface Synthesis of Nitrogen-Doped Kagome Graphene

Rémy Pawlak,* Xunshan Liu, Silviya Ninova, Philippe D'Astolfo, Carl Drechsel, Jung-Ching Liu, Robert Häner, Silvio Decurtins, Ulrich Aschauer, Shi-Xia Liu,* Ernst Meyer,* *Angew. Chem. Int. Ed.* 2021, *60*, 8370-8375,
https://doi.org/10.1002/anie.202016469.
University of Bern, University of Basel

Nitrogen-doped Kagome graphene (N-KG) has been theoretically predicted as a candidate for the emergence of a topological band gap as well as unconventional superconductivity. The authors report on the substrate-assisted reaction on Ag(111) for the synthesis of two-dimensional graphene sheets possessing a long-range honeycomb Kagome lattice. The use of linear ditopic molecules leads first to an organometallic intermediate which further transforms to a covalent Kagome-type structure consisting of a regular pattern of triangular nodes. Incorporation of pyrazine units into the pentacene-type precursor molecule leads to an atomically precise N-doping of the extended monolayer structure. Low–temperature scanning tunneling microscopy (STM) and atomic force microscopy (AFM) with a CO-terminated tip supported by density functional theory are employed to scrutinize the structural and electronic properties of the N-KG down to the atomic scale. The semiconducting character due to the nitrogen doping as well as the emergence of Kagome flat bands near the Fermi level which would open new routes towards the design of graphene-based topological materials is demonstrated.

Authors' comments:
"The specific design of a Br-functionalized tetraazapentacene derivative was key to the successful bottom-up synthesis of porous graphene sheets with atomically precise N-doping. The combination of on-surface preparative techniques under ultrahigh vacuum conditions with analytical scanning probe methods allowed to map the local physical properties down to the nanoscale."