Q: how would one incorporate Inchi into a ML workflow. Assuming we start with a large set of Inchi representation, can we tranform these into structural descriptors (something like SOAP) that then can be used for ML modeling and predictions?

A: A large set of InChI is an ideal starting point for sn ML workflow. The InChI makes it easy to remove any duplicates (including variant guanine structures and other tautomers) and to check that any new entries to the database are unique. Most chemistry toolkits will read in InChI and use them to generate structure descriptors suitable for ML modelling and predictions. (JG)

Q: Is the InChI software free for all users?

A: The InChI software is open source and free. Download from: https://github.com/IUPAC-InChI

Q: How do you see InChI and chemical informatics contributing to the discovery and optimization of advanced functional materials in the future?

A: The InChI is a useful tool for all studies based on molecular structures, including advanced functional materials

Q: can InChI be applied for transition metals compounds alone? And can InChI be applied for transition metal ligands attached to organic compounds?

A: The current standard InChI v1.07 can encode transition metals and ligands attached to transition metals but is probably not quite precise enough for all applications as it does not encode most metal-carbon bonds. The current behaviour is useful for some applications. However, a fuller description of structures including transition metals is being developed. The InChI Web Demo lets you experiment with this if you switch the version to “Dev with Molecular Inorganics”.