Contribution ID: **36**   Type: **not specified**

AI Tools that Auto-generate Materials Databases for Building Data-science Platforms

Monday, 18 October 2021 14:50 (20 minutes)

This presentation will introduce and exemplify the artificial intelligence tools that my group have been developing with ISIS. These use data-mining and machine-learning methods to build data-science platforms that aid materials characterisation and materials application methods. These include the incorporation of neutron scattering data. I will also show some examples of how these data-science platforms can lead to the data-driven prediction and discovery of new materials.

References to our AI tools
[1] Swain and Cole, J. Chem. Inf. Model. 2016, 56, 10, 1894–1904 www.chemdataextractor.org
[2] Mavracic, Court, Isazawa, Elliott, Cole, J. Chem. Inf. Model. 2021, 61, 9, 4280–4289 www.chemdataextractor2.org
[3] Yildirim, Cole, J. Chem. Inf. Model. 2021, 61, 3, 1136–1149 and Mukaddem, Beard, Yildirim, Cole, J. Chem. Inf. Model. 2020, 60, 5, 2492–2509 www.imagedataextractor.org
[4] Wilary and Cole, J. Chem. Inf. Model. 2021, https://doi.org/10.1021/acs.jcim.1c01017 www.reactiondataextractor.org

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Session Classification: New algorithms and Machine learning: relevance to inelastic neutron scattering (Chair: Toby Perring)