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Contribution ID: **95** Type: **Talk**

The degradation of phosphate derived ligands in hydrometallurgical solvent extraction

Wednesday, 6 December 2017 14:10 (20 minutes)

HPC content

The work that will be presented was done using the DMol3 code as implemented in BIOVIA's Materials Studio (2016 version) computational chemistry software package. Most of the calculations were done using the CHPC's Lengau cluster, to which calculations were submitted in such a way that 24 to 72 cores were used per calculation.

Primary author: Mr JANSEN VAN VUUREN, Daniel (North-West University)

Co-authors: Dr VAN SITTERT, Cornie (North-West University); Mr VAN DER WESTHUIZEN, Derik (North-West University); Prof. KRIEG, Henning (North-West University)

Presenter: Mr JANSEN VAN VUUREN, Daniel (North-West University)

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