



Contribution ID: 95

Type: **Talk**

The degradation of phosphate derived ligands in hydrometallurgical solvent extraction

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

CHPC 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.

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Session Classification: Chemistry

Track Classification: Materials Science & Physics