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COMSOL Multiphysics Programming Reference Manual

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TheAlloy-TheoreticAutomatedToolkit(ATAT):AUserGuide

Chapter 2 Credits and Licence The Alloy-Theoretic Automated Toolkit (ATAT)¹ is a generic name that refers to a collection of alloy theory tools developed by Axel van de Walle², in collaboration with various research groups. 2.1 Collaborators and Credits The MAPS3 (MIT Ab-initio Phase Stability) code, which automatically constructs a cluster expansion from the

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