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Vysoká škola chemicko-technologická v Praze (University of Chemistry and Technology, Prague) ¹

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xxxxx, Group of Computational Thermodynamics, Dep. of Physical
Chemistry.....²

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"The calculations have been performed using the Vienna ab-initio simulation package VASP.X.x [1,2]."

[1] xxxxx and xxxxx, Phys. Rev. B **54**, 11 169 (1996).

If the PAW potentials are used, reference shall be made to

[2] xxxxx and xxxxx, Phys. Rev. B **59**, 1758 (1999).

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said provision eliminated. The invalid provision shall be replaced by a provision which comes as close as possible to the will of the parties within the framework of what is legally possible and which best corresponds in its economic effect to the invalid provision.

For the VASP Software GmbH:

XXXXX

Sensengasse 8, A-1090 Wien, Austria

Signature and Date: 2.8.2021

For the Licensee

XXXXX, bursar

Name and capacity in which acting:

Vysoká škola chemicko-technologická v Praze (University of Chemistry and Technology, Prague)

Institution:

Technická 5, 16628 Praha 6, Czechia

Address of Institution:

Signature and Date: 22.7.2021

The research group leader and the primary-contact-person responsible for the installation of VASP herewith confirm that they have read the contract in full. They understand that under this license access to VASP is restricted to 6 named users and that the password to the VG download account must not be shared with anyone for whatsoever reason.

For the research group entitled to use VASP

Research group:

XXXXX, Group of Computational Thermodynamics, Dep. of Physical Chemistry

Address of Research group:

Vysoká škola chemicko-technologická v Praze (University of Chemistry and Technology, Prague), Technická 5, 16628 Praha 6, Czechia

Name:

XXXXX

Signature and Date: 22.7.2021

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Primary-contact-person responsible for the installation of VASP at the institution
(leave blank, if the primary contact-person and the signatory for the research group are identical)

Name: xxxxx

Signature and Date: 22.7.2021