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Harvard University  
Accounts Payable  
PO Box 381588  
Cambridge, MA 02238  
USA  
Attn.: Ms. Anna Shin

Invoice Nr. 5-1225  
Your Purchase Order Nr. 70000328675

Academic license for the research group of Dr. Alán Aspuru-Guzik at the Department of Chemistry and Chemical Biology of the Harvard University, at 12 Oxford Street, Cambridge, MA 02138, USA, to VASP.5.2, as described in the agreement between the two institutions.  
The Terms of the License agreement override all Terms and Conditions of the Purchase Order.

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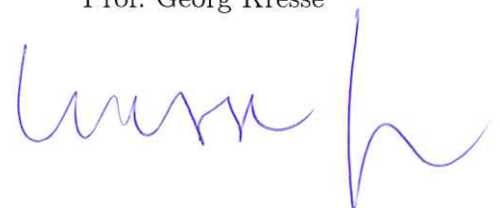
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Wien, March 26<sup>th</sup>, 2012

for the Universität Wien  
Prof. Georg Kresse



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[1] G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11 169 (1996).

If the PAW-version is used, reference will be made to

[2] G. Kresse and D. Joubert, Phys. Rev. **59**, 1758 (1999).

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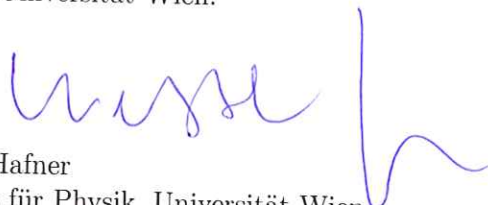
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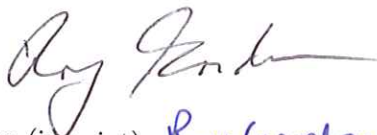
For the Universität Wien:



Jürgen Hafner  
Fakultät für Physik, Universität Wien  
Sensengasse 8/12, A-1090 Wien, Austria

Date March 26th, 2012

For the President &amp; Fellows of Harvard College (Harvard University)



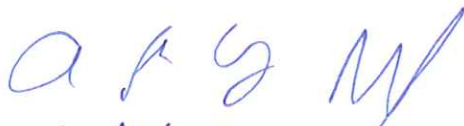
Name (in print): Roy Gordon

Institution: Department of Chemistry &amp; Chemical Biology, Harvard University

Address: 12 Oxford Street, Cambridge, MA 02138, USA

Date 3/22/12

For the research group entitled to use VASP5.2: Aspuru-Guzik Group



Name (in print): Alán Aspuru-Guzik



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Created by Email	anna@chemistry.harvard.edu
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1	Supplier Item: VASP 5.2 software license (4,000.00 EUR = estimated \$5,252.36 USD) for Synthesis of Electrocatalytic Oxides Enabling Grid-Scale Electricity Storage proj	5252.36	Each	1.00	5,252.36
Note to Supplier: Please mail invoice to Anna B. Shin, Aspuru-Guzik Group, Chemistry & Chemical Biology, Harvard University, 12 Oxford Street, Cambridge MA 02138, USA.					
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