

## VASP Survey (Nov. 19, 2008)

### Groups who have ever run/tried VASP on SHARCNET clusters

[7 groups, 4 licenses, one did not response, only the York groups (share a license) run lots of VASP jobs on SHARCNET clusters]

Status	Name	Sharc net ID	Email	Site	Research Area	License
Student	Fatih Sen	fatih	senf@uwindsor.ca	Windsor		
PI	Ahmet T.Alpas	aalpas	aalpas@uwindsor.ca	Windsor	Materials Science and Engineering	yes
Student	Anna Sankari	sankari	ans341@mail.usask.ca	U. Saskatchewan		
PI	John Tse	jtse	John.Tse@usask.ca	U. Saskatchewan	Condensed Matter Physics	no response
Student	Chi Kit Siu	cksiu	cksiu@yorku.ca	York Univ	Chemistry	
PI	Michael Siu	kwmsiu		York Univ		yes
Student	Min Zhang	zhangmin	zhangmin@yorku.ca	York Univ.		
PI	Rene Fournier	renef	renef@yorku.ca	York Univ	Chemistry	yes, shared with M. Siu
Student	Abu Asaduzzaman	asaduzza	asaduzza@cc.umanitoba.ca	Univ. Manitoba		
PI	H. Georg Schreckenbach	schrecke	schrecke@cc.umanitoba.ca	Univ Manitoba	Chemistry	yes
Student	Isaac Tamblyn	itamblyn	itamblyn@dal.ca	Dalhousie		
Student	Amanuel Teweldeberhan	amanuel	a.m.teweldeberhan@dal.ca	Dalhousie		
PI	Stanimir Bonev	bonev	stanimir.bonev@dal.ca	Dalhousie	Condensed Matter Physics	no, intend to get a license
Student	James Hooper		jhoop018@uottawa.ca	U. Ottawa		
PI	Tom Woo	twoo	twoo@uottawa.ca	Univ Ottawa	Chemistry	yes

## Response from PIs (until Nov. 28, 2008)

[15 groups showed interests, 5 groups purchased the VASP group license, 2 groups intend to buy, 2 groups (Ralf Meyer at Laurentian and David Shoosmith at UWO) made the request recently]

Name	Dept	Institution	S-ID	license	Interest
Martin Muser	Applied Maths	UWO	muser	no	yes
Clara Wren, David Shoosmith	Chemistry	UWO	jcwren	no	<b>Yes</b>
Viktor N. Staroverov	Chemistry	UWO	vstarove	no	yes
Nick Mosey	Chemistry	Queen's University	njmosey	no	yes
Marek Niewczas	Materials Science & Engineering	McMaster University		no, intend to buy one	yes
Paul Ayers	Chemistry	McMaster	ayers	no	yes
Jeffrey J.Hoyt	Materials Science and Engineering	McMaster	jjhoyt	no	yes
Vesselin Stoilov	Mechanical, Automotive and Materials Engineering,	Univ. Windsor	vstoilov	<b>Yes</b>	yes
Fatih Sen/ Ahmet T.Alpas	Materials Science and Engineering	Windsor	Faith, aalpas	<b>Yes</b>	yes
James Gauld	Chemistry	Windsor	jgauld	no	yes
Micheal Siu/Rene Fournier	Chemistry	York U	Kwmsiu, renef	<b>Yes, joint license</b>	<b>Yes</b>
Georg Schreckenbach	Chemistry	U. Manitoba		<b>Yes</b>	yes
Ralf Meyer	Mathematics and Computer Science	Laurentian	rmeyer	no	<b>Yes</b>
Tom Woo	Chemistry	Ottawa	twoo	<b>Yes</b>	<b>Yes</b>
Stanimir Bonev	Condensed Matter Physics	dalhousie	bonev	no, intend to buy one	yes

**Inquiry email sent to ~130 PIs in the research areas of Chemistry, Biochemistry, Molecular simulation, Molecular Dynamics, Materials Simulation, and Condensed Matter Physics**  
(Nov. 19, 2008)

Dear Professors,

Recently a few professors reached SHARCNET to run VASP on SHARCNET clusters. VASP is a package for performing ab-initio quantum-mechanical molecular dynamics (MD) using pseudopotentials and a plane wave basis set. It is a commercial software and the license is issued to individual research group. VASP's homepage can be found from <http://cms.mpi.univie.ac.at/vasp/>

Our job records show that some of you have run your group VASP license on SHARCNET clusters. It maybe possible for SHARCNET to get a copy of VASP if there is a large number of licensed VASP groups on SHARCNET.

We hope to know how many of you have purchased the VASP license already and how many of you are interested in VASP.  
Please reply this email in the format

Your name, Department, Institution, Sharcnet ID, VASP license (Yes/no, interested/not)

Based on your replies, we may talk to VASP for possible solution.  
If you are not interested in VASP, please ignore this email.

Thank you very much for your times.

Regards,  
Jemmy

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Jemmy Hu                    SHARCNET  
HPC Analyst                University of Waterloo  
(519)888-4567 x37854      PHY-2008  
jemmyhu@sharcnet.ca      <http://www.sharcnet.ca>

**Another email sent to PIs, and CCed to those students who have run/ried VASP on SHARCNET to confirm whether they own a VASP license**

Dear Professors,

SHARCNET job records show that your group (your students CCed in this email) have run VASP on SHARCNET clusters in the past or current.

VASP is licensed to individual group. There is no campus or site license, or HPC center license. However, if a significant number of SHARCNET user groups own the VASP license, we could be able to ask for a copy of VASP for SHARCNET, which will enable your group to run VASP more efficiently.

The purpose of this email is to confirm how many groups own a VASP license. Could you please reply my email to confirm that your group own a VASP license?

Please allow me to list the students who have run/tried VASP on SHARCNET:

Student	Supervisor
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Fatih Sen	Ahmet T.Alpas
Anna Sankari	John Tse
Chi Kit Siu	Michael Siu
Min Zhang	Rene Fournier
Abu Asaduzzaman	H. Georg Schreckenbach
James Hooper	Tom Woo
Isaac Tamblyn	Stanimir Bonev
Amanuel Teweldeberhan	Stanimir Bonev
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Thank you very much for your times

Regards,  
Jemmy