

**Jemmy Hu, November 04, 2011**

Emailed to PIs in Sharcnet Gaussian user group on Oct. 31, 2011

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Dear All,

Some of you may have heard of Turbomole, another computational chemistry software. It's a commercial software from Cosmologic, Germany.

<http://www.cosmologic.de/index.php>

SHARCNET wants to know

- 1) Have you purchased the license of Turbomole?
- 2) Have you ever run your Turbomole software on SHARCNET systems?
- 3) Are you interested in using Turbomole for your researches, for real?

If you do not hear about it, or you do not use it for real in the near future, please ignore this email.

Thanks,

Jemmy

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**Responses from PIs (9)**

Name, Institution	Responses	Interested?
Paul Ayers McMaster	I know the software and I think it is good. If it were available, we would use it some. That said, I think Molpro and Orca are better packages. Turbomole is, to my mind, less innovative than those programs. [The program is definitely faster, but it has fewer features. There is more innovation in Orca and Molpro than Turbomole, which is slowly becoming rather stagnant. I'm not sure how widely either Turbomole or Molpro is used; in Europe they are very popular, but less-so in North America.	yes?
James Gauld Windsor	We do not have it, nor used it before. But if you buy it - we might use it. For real.	Yes
Yining Huang UWO	I have no need for this particular software, but was wondering if there are funds available for purchasing certain software.	no
Peter Guthrie UWO	I am interested in solvation energy calculations using the cosmologic software (turbomole with cosmo-RS), but have not done any of these calculations. If it were available on sharcnet I would use it.	Yes
John Goddard Guelph	We purchased a license for Turbomole some years ago (probably 2006 it has probably expired and I am sure there are new releases). It was set it up on SHARCnet. It was one of the first programs to have excited state gradients with TDDFT.	Not anymore?
Travis Dudding Brock	I know about this program and would be interested in using. Unfortunately, however I've not had much experience with using due to its cost.	Yes
Terry McMahan UW	We have not purchased Turbomole license here at Waterloo but we have used it in collaboration with a research group at Ecole Polytechnique in France. It runs much faster than Gaussian in general. We would definitely be interested in having it available on Sharcnet.	YES
Barry Lever York	I have not used it, but I would use it if it were available on Sharcnet - for comparison with Gaussian	yes?
Scott Hopkins UW	Yes, I would like to use Turbomole for my researches	YES

**\*Two UW PIs are definitely interested in it, Five others showed interests if it's available, Two said no.**