

THE SUPER COMPUTING SCIENCE CONSORTIUM

Pennsylvania-West Virginia
partners in development of clean
power technologies.

Formed in 1999 and supported by the U.S. Department of Energy, the Super Computing Science Consortium is a regional partnership of research and educational institutions in Pennsylvania and West Virginia. (SC)² provides intellectual leadership and advanced computing and communications resources to solve problems in energy and the environment and to stimulate regional high-technology development.

Through (SC)², Evergreene Technology Park in Greene County provides a channel for companies to collaborate with local universities in southwest Pennsylvania and West Virginia and to have access to PSC computing resources.

Since the spring of 2000, a high-speed network — the first fiber-optic service to Morgantown, West Virginia — has linked the National Energy Technology Laboratory (NETL) campuses in Morgantown and Pittsburgh with PSC, facilitating NETL collaborations. Researchers at NETL and WVU have actively used this link to tap PSC computational resources. Since the founding of (SC)², 45 (SC)² researchers have used PSC systems for a range of projects, using more than three million hours of computing time, nearly 400,000 hours within the past year. This work includes:

- ♦ *Gas From Black Liquor*
<http://www.psc.edu/science/2004/sc2/>
- ♦ *Fluidized-Bed Combustion of Silane*
<http://www.psc.edu/publicinfo/netl/>
- ♦ *Lean-Fuel Mixes in Next-Generation Power-Generating Turbines*
http://www.psc.edu/science/Richards/clean_power.html
- ♦ *Industrial-Scale Technology for Coal Gasification*
<http://www.psc.edu/publicinfo/2002/sc2/>
- ♦ *A New Design for a Power-Generating Turbine*
<http://www.psc.edu/science/cizmas2002.html>
- ♦ *How to Produce Fuel-Quality Hydrogen*
<http://www.psc.edu/science/2005/sc2>

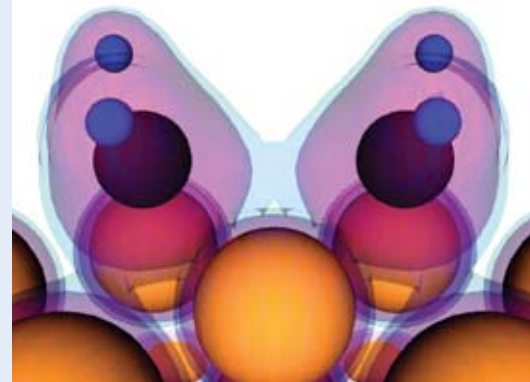


(SC)² PARTNERS

National Energy Technology Laboratory
Pittsburgh Supercomputing Center
Carnegie Mellon University
Duquesne University
University of Pittsburgh
Waynesburg College
West Virginia University
Institute for Scientific Research
NASA Independent Verification & Validation
Facility
The West Virginia Governor's Office of
Technology

More Information

<http://www.sc-2.psc.edu>



Clean Liquid Fuel

Fischer-Tropsch synthesis (FTS) is an important industrial process that offers a direct route to produce clean hydrocarbon liquid fuel from syngas (a mixture of carbon monoxide and hydrogen). Traditionally coal or natural gas have been used as feedstocks but biomass-derived hydrogen also could work, offering promise for a liquid fuel to replace fuels produced from petroleum or other fossil fuels.

With support through NETL, Manos Mavrikakis and colleagues at the University of Wisconsin, Madison apply advanced quantum-mechanical computations at PSC to gain insight into the FTS reaction. This graphic shows the "transition state" in the formation of ethylene (C₂H₄, enclosed by two electron density surfaces) on a catalytic surface of iron (orange atoms) where the carbon-carbon bond (two dark spheres) is formed.

"Experimental techniques can't provide information about transition states," says Mavrikakis, "and computational methods are the only means to study them."



(SC)² co-chairs **Lynn Layman** of PSC (left) and **Bob Romanosky** of NETL on July 14 at Waynesburg with **Pennsylvania Governor Ed Rendell** and members of the event's planning team, (l to r) **Paul Cizmas** of Texas AGM, **Trina Waffle** of WVU, **Governor Rendell**, **Francis Van Scoy** of WVU, **Barbara Kirby** of Waynesburg College, **Robin Flaus** of PSC, **Tom Maiden** of PSC, **Laura McGinnis** of PSC, and **Don McLaughlin** of WVU.



The seminar included a poster session presenting research by students from regional colleges, including West Virginia University, Waynesburg College, the University of Puerto Rico, the University of Pittsburgh, Penn State, the University of Miami, Cornell University, Alderson Broadus College and a K-12 project from ASSET.



The keynote speech by **Stephen Meacham**, Program Director, Office of Cyberinfrastructure, National Science Foundation, highlighted high-end computing as an engine for competitiveness. "What the Supercomputing Science Consortium has done," he said, "is show how you can leverage the investment of the National Science Foundation by pulling together universities with local development opportunities. It represents a microcosm of how society can be transformed by investment."

Regional Business Opportunities in Supercomputing

Economic development was the theme of this July 14 (SC)² seminar. Sponsored by PSC, a founding partner in (SC)², and held at Waynesburg College, the event offered a learning opportunity aimed at small-to-medium-sized technology-oriented organizations.

Governor Ed Rendell spoke during an afternoon panel discussion on "Federal, State and Other Funding Opportunities for Regional Small Businesses, Colleges and Universities." He stressed the importance of a skilled workforce for economic growth. The Pennsylvania economy, he said, must compete not only against other states, but also increasingly against corporations around the world and as far away as Singapore. "The currency of where growth will occur in our new economy," said Rendell, "lies with innovation and the availability of a skilled work force."

Participants in the panel were Errol Arkilic, Program Manager, Small Business Innovation Research and Small Business Technology Transfer Programs, National Science Foundation; Chris Gabriel, Innovation Economy Program Director, Heinz Endowments; Brian Kennedy, Government Relations Director, Pittsburgh Technology Council; Paul Hill Jr., Executive Director, West Virginia EPSCoR, and Susan Zelicoff, of the Institute for Entrepreneurial Excellence at the Katz Graduate School of Business, University of Pittsburgh.