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COMPUTER FOR AB INITIO MOLECULAR DYNAMICS SIMULATIONS

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13. ABSTRACT *(Maximum 200 words)*

This DURIP funding was used to contribute to the expansion of an IBM SP parallel computer and its support hardware. This computer resource is being utilized for the computationally demanding ab initio molecular dynamics simulations that are part of the P.I.'s ONR funded research program. The goal of this program is to compute realistic rates for electrochemical reactions. The simulations are extraordinarily demanding in CPU time and memory requirements and have begun to yield very important new results for the water/metal electrode interface.

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Final Technical Report
ONR DURIP Grant N00014-98-1-0323
PR Number 98PR04001-00

Equipment Acquired by Name, Manufacturer, and Cost:

8-node SP system	IBM	$99,000
Two Origin 200 Servers	Silicon Graphics	$18,126
One 9mm exabyte tape drive	Ramsys	$1,323
Two 18 Gbyte disk drives	Ramsys	$2,176
Repair and maintenance	Silicon Graphics	$365
Total		$121,170

Special Circumstances:

The equipment purchased deviated only slightly from the original proposal in that the $121,170 provided by the ONR DURIP grant was used to leverage and addition $333,000 from the University of Utah to add eight, instead of four, nodes to the IBM SP system, and to double the memory on each node. One Silicon Graphics Origin200 server was purchased to help provide local data storage which could not be accommodated on the SP, and one half of another SGI Origin200 was purchased to provide graphical analysis of the data produced by the simulations on the SP. A 9mm exabyte tape drive was purchased for back-up purposes, and two 18 Gbyte disk drives were purchased for the SGI server to expand disk storage capacity.

Use of the Equipment:

The research usage of the equipment purchased conforms to that which was described in the original DURIP proposal as funded by ONR. Briefly, we are carrying out the first fully *ab initio* simulations of the water/metal interface. These simulations show that significant coupling between solvent molecules and surface states can occur even in the presence of a disordered solvent. This coupling is expected to have significant effects in heterogeneous electron transfer between the solid and aqueous redox species because the solvent-surface electronic coupling facilitates the transport of electron density away from the surface. In turn, the electron exchange between the solid and redox species is also coupled to specific solvent fluctuations in a non-trivial way. By combining the information obtained from these simulation with largescale classical molecular dynamics simulations using the appropriate effective Hamiltonians developed in our group, the accurate calculation of heterogeneous electron transfer rates for realistic systems will become a reality.