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Surface and Defects Excitations in Covalently Bonded Solids

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Work by Prof. Joannopoulos and his collaborators is summarized here

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IN COVALENTLY BONDED SOLIDS

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- a. Number of Papers Submitted to Refereed Journals but not yet published: 0
- b. Number of Papers Published in Refereed Journals: 10 (List Attached)
- c. Number of Books or Chapters Submitted but not yet Published: None
- d. Number of Books or Chapters published: None
- e. Number of Printed Technical Reports & Non-Refereed Papers: None
- f. Number of Patents filed: 1
- g. Number of Patents Granted: None
- h. Number of Invited Presentations at Workshops or Prof. Society Meetings: 7 (List Attached)
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- j. Honors/Awards/Prizes for Contracts/Grant Employees: 4 (List Attached)
- k. Total Number of Graduate Students and Post-Docs Supported at least 25% this year on this contract grant:

Grad Students 1 and Post Docs 1
Grad Student Female 0
Grad Student Minority 0
Grad Stud. Asian e/n 1
Post-Doc Female 0
Post-Doc Minority 0
Post-Doc Asian e/n 0

(b) Publications in Refereed Journals

1. A. Rappe, K. Rabe, E. Kaxiras and J.D. Joannopoulos, "Optimized Pseudopotentials," Phys. Rev. Rapid Comm. **B41**, 1227 (1990).
2. M. Payne, E. Tarnow, P. Bristowe and J.D. Joannopoulos, "Ab-initio Materials Science and Engineering Using the Molecular Dynamics Methods for Total Energy Pseudopotential Calculations," Molecular Simulations **4**, 79 (1990).
3. M. Needels, J.D. Joannopoulos, S. Pantelides and Y. Bar-Yam, "Oxygen Complexes in Si," Phys. Rev. **B43**, 4208 (1991)
4. M. Needels, J.D. Joannopoulos, Y. Bar-Yam and S. Pantelides, "The Enchanting Properties of Oxygen Atoms in Silicon," Mat. Res. Soc. Proc. **209**, 103 (1991)
5. R. Wolfe, M. Needels and J.D. Joannopoulos, "The Electronic Struture of Oxygen in Silicon as Revealed by Volume Visualization of Ab-Initio Calculations," Proc. IEEE Conf. "Visualization '91", San Diego (1991), in press.
6. R.D. Meade, K.D. Brommer, A.M. Rappe and J.D. Joannopoulos, "Photonic Bound States in Periodic Dielectric Materials", Phys. Rev. Rapid Comm. in press (1991).
7. T. Arias, M. Payne and J.D. Joannopoulos, "Precise and Efficient Ab-Initio Molecular Dynamics," Phys. Rev. B in press (1991).
8. E. Yablonovitch, T. Gmitter, R. Meade, A. Rappe, K. Brommer, and J.D. Joannopoulos, "Donor and Acceptor Modes in Photonic Band Structures" Phys. Rev. Lett. **67**, 3380 (1991)
9. A. Rappe and J.D. Joannopoulos, "The Desigr. of Convergent and Transferable Ab-Initio Pseudopotentials", Proc. Nato Adv. Study Inst., Aussois, France (1991), Vol **205**, p. 409
10. J.D. Joannopoulos, P. Bash and A. Rappe, " Modern Iterative Minimization Techniques in Quantum Chemistry", Chemical Design Automation News, Aug. (1991).

(h) Invited Papers

1. J.D. Joannopoulos and A. Rappe, NATO Adv. St. Inst., "Computer Simulation in Material Science", Aussois, France (1991).
2. J.D. Joannopoulos, "Physics Computing '91", Bull. APS (1991).
3. R. Meade, K. Brommer, A. Rappe and J.D. Joannopoulos, Proc. Prog. Elect. Res. Symposium, Cambridge (1991).
4. R. Meade, A. Rappe, K. Brommer and J.D. Joannopoulos, Amer. Optical Soc. Meeting, San Jose (1991).
5. T. Arias. (J.D. Joannopoulos, M. Payne), Total Energy Workshop, Trieste (1991).
6. J.D. Joannopoulos, Gordon Conference on Adhesion (1991).
7. J.D. Joannopoulos, Workshop on Epitaxy, Interfaces and Defects, Pittsburgh (1991).

(j) Honors, etc.

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|----------------------|----------------------------------|
| 1. John Joannopoulos | School of Science Teaching Award |
| 2. Andrew Rappe | JSEP Fellowship |
| 3. Tomas Arias | AT&T Bell Labs Fellowship |
| 4. Kyeongjae Cho | Korean Overseas Scholarship |

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