Prof. Thonhauser

Theoretical Condensed Matter Physics
Computational Materials Science

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e-mail: thonhauser@wfu.edu
phone: (336) 758 3991

Research

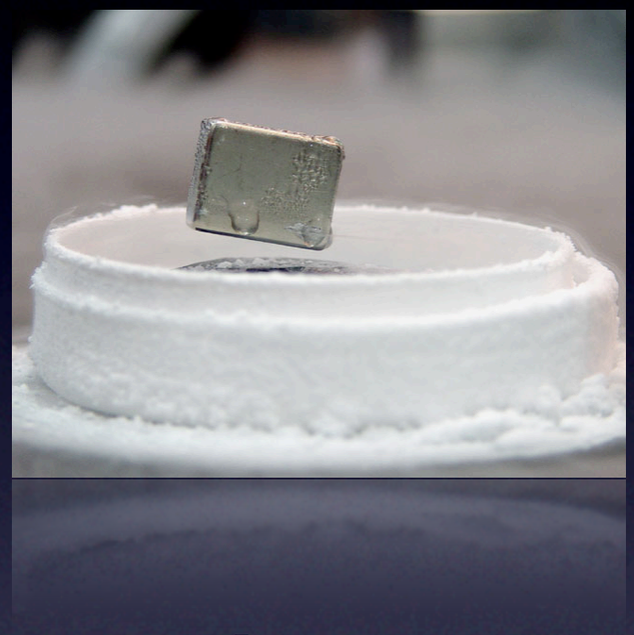
? magnetic properties

? mechanical properties

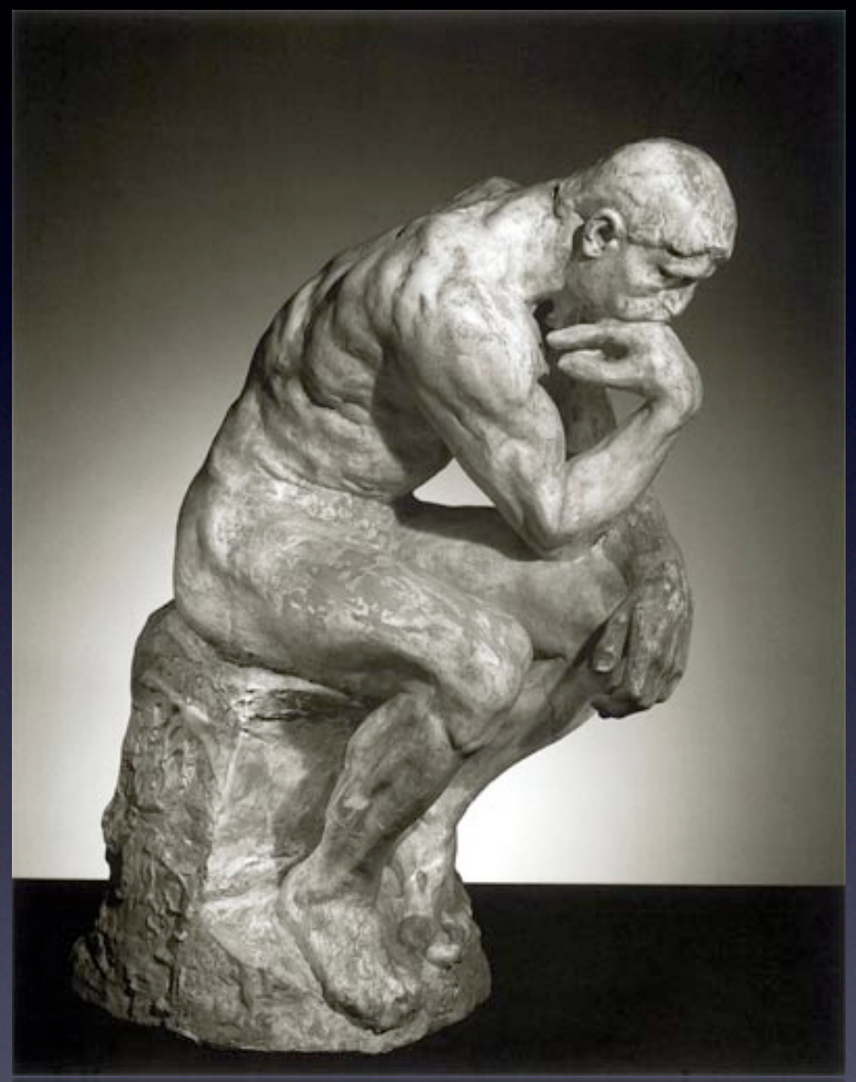
? electrical properties

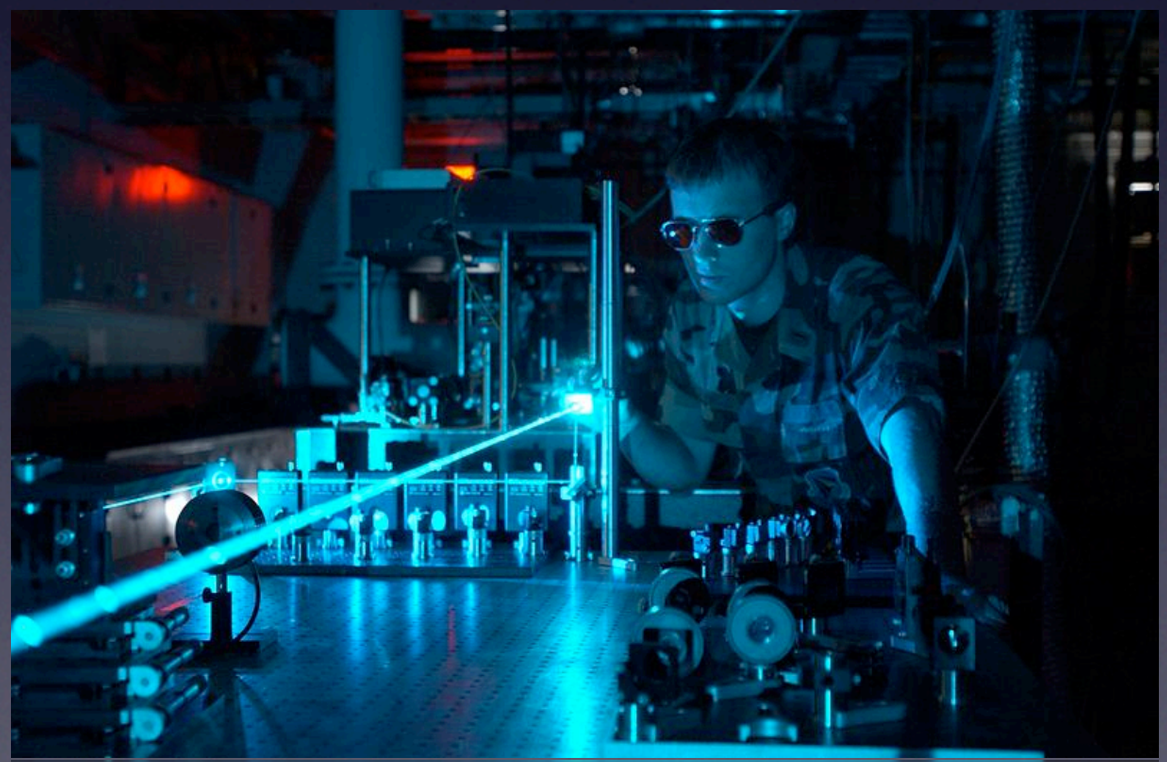
? optical properties

Because everything is a material ...



Theory vs. Experiment





Pencil & Paper vs. Computer

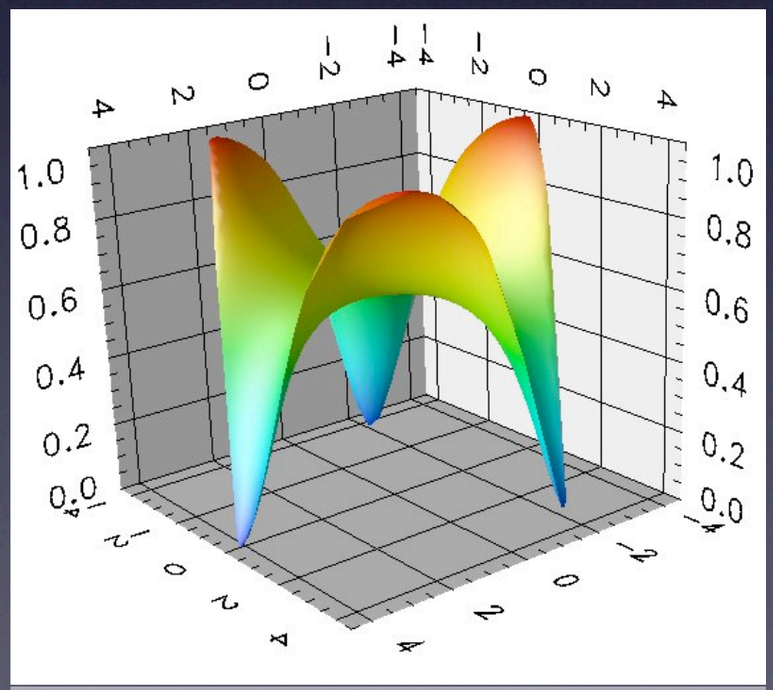
Pencil & Paper vs. Computer

PHYSICAL REVIEW LETTERS

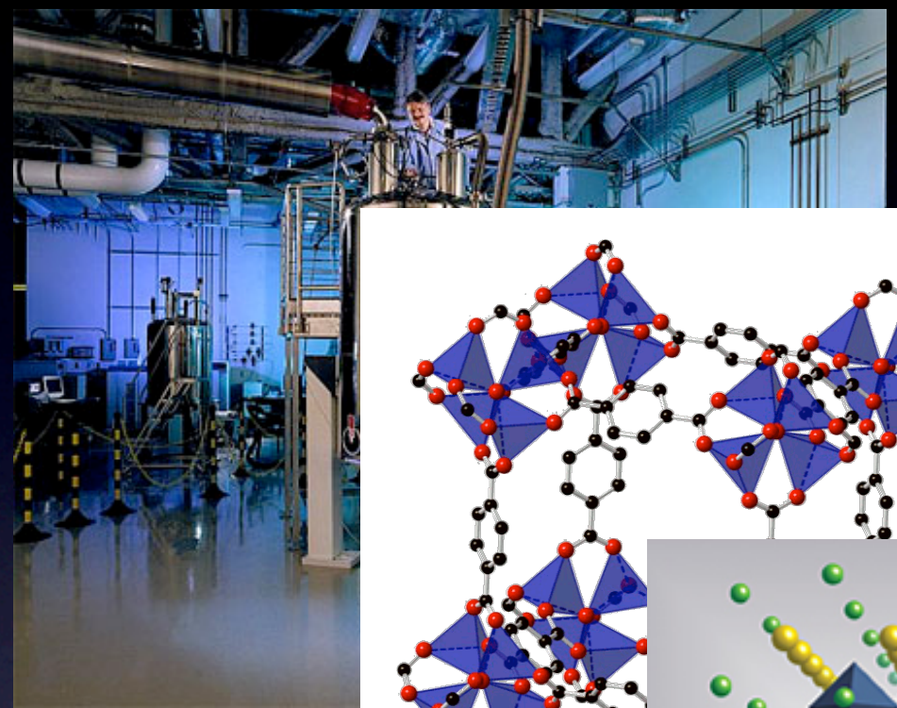
Orbital Magnetization in Periodic Insulators

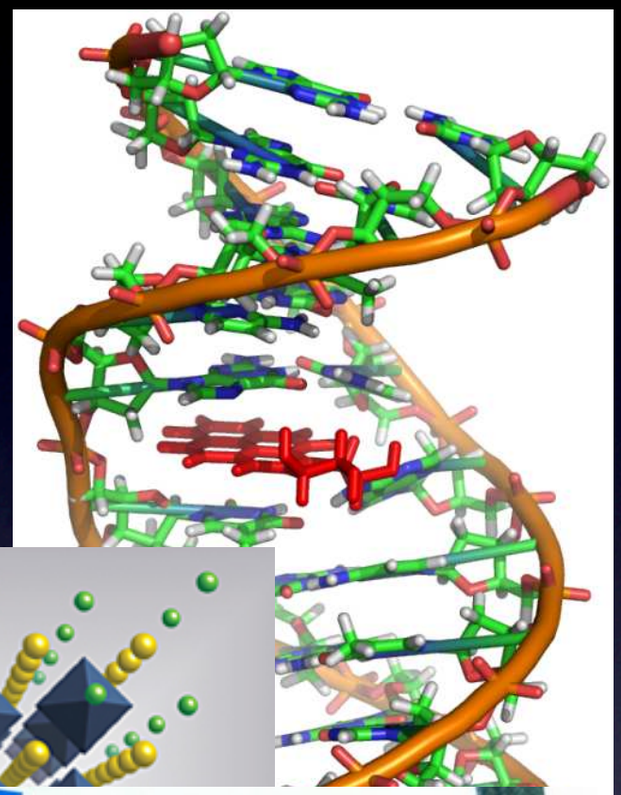
T. Thonhauser,[1] Davide Ceresoli,[2] David Vanderbilt,[1] and R. Resta[3]
ıent of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08
ol for Advanced Studies (SISSA/ISAS) and INFM-DEMOCRITOS, via Beirut 4,
ca Teorica Università di Trieste and INFM-DEMOCRITOS, strada Costiera 1
(Received 20 May 2005; published 22 September 2005)

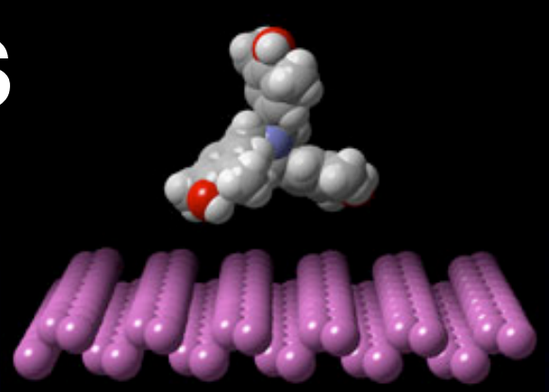
in the Wannier representation, we derive an expression for the orbital magn
ulator. The magnetization is shown to be comprised of two contributions, an
ith the internal circulation of bulklike Wannier functions in the interior, and a
from net currents carried by Wannier functions near the surface. Each contrib
s a bulk property in terms of Bloch functions in a gauge-invariant way. Our
comparing numerical tight-binding calculations for finite and periodic samples.

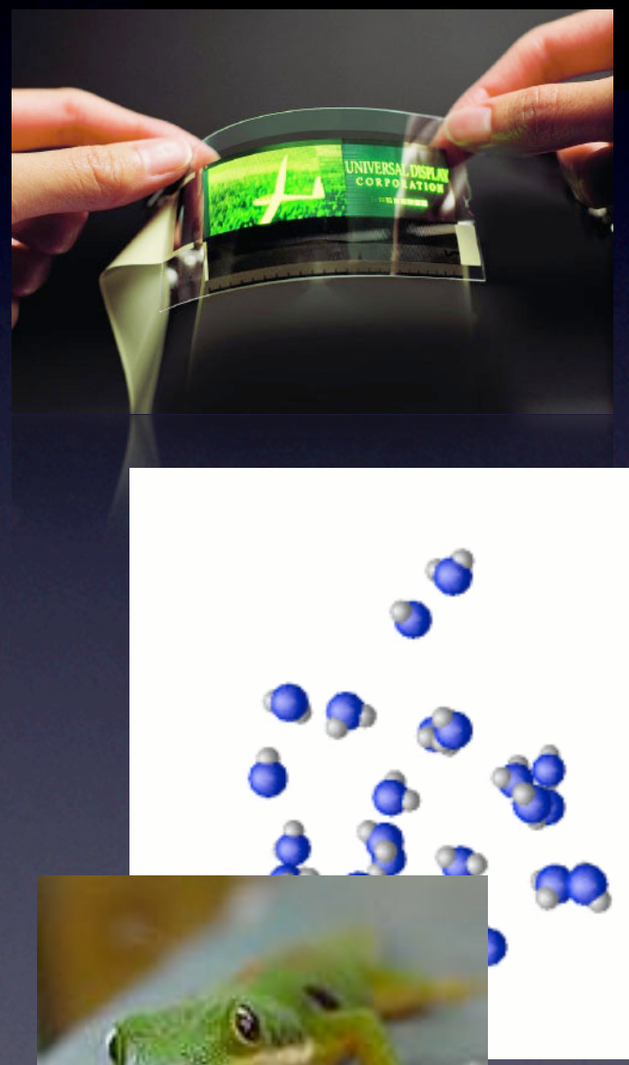


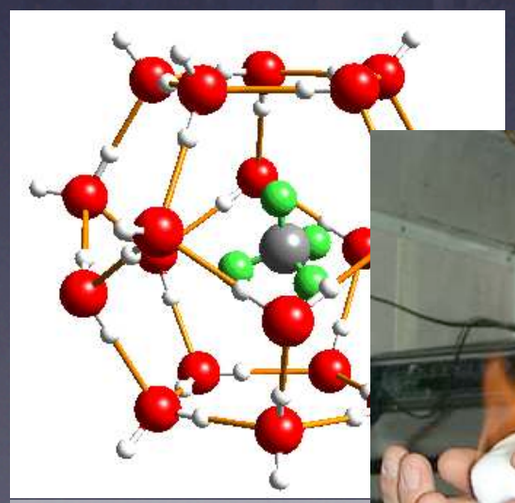
Ongoing and Future Projects











Help Wanted ... Apply Here!

Undergraduate & Graduate Students needed who have an interest in ...

- Condensed matter physics
- Materials science
- Quantum mechanics
- Computers - Linux/Unix
- Programming C++, Fortran

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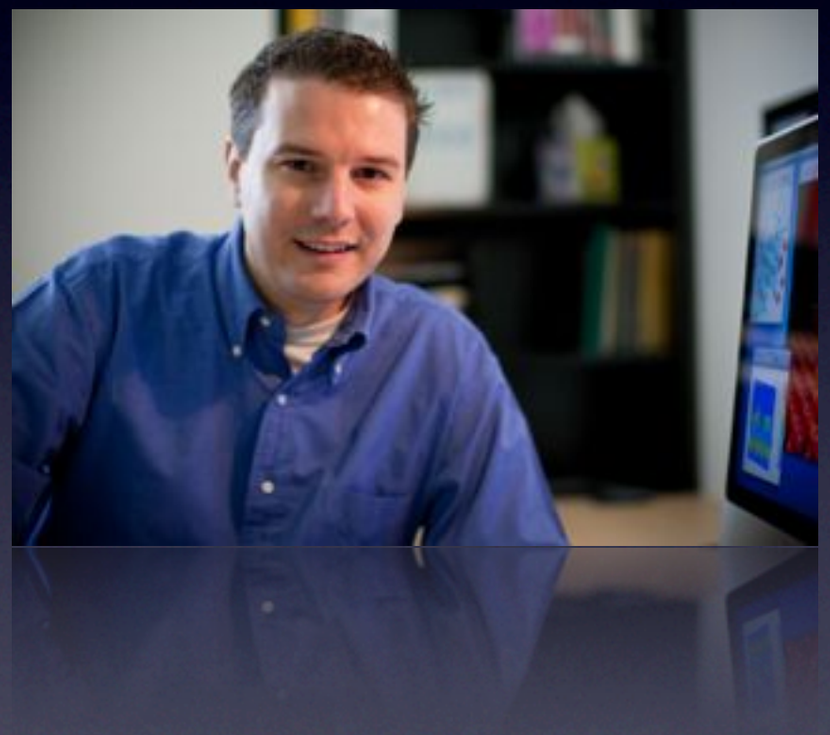
- Quantum mecha
- Computers - Lin
- Programming C-

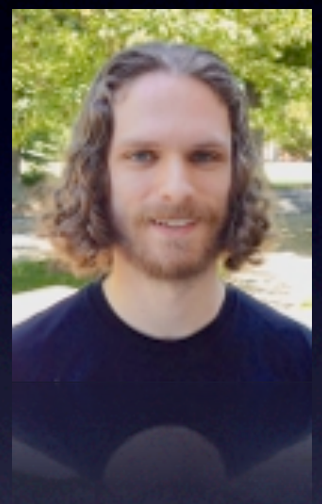
Two fully funded RA positions for 5 years!

The Group

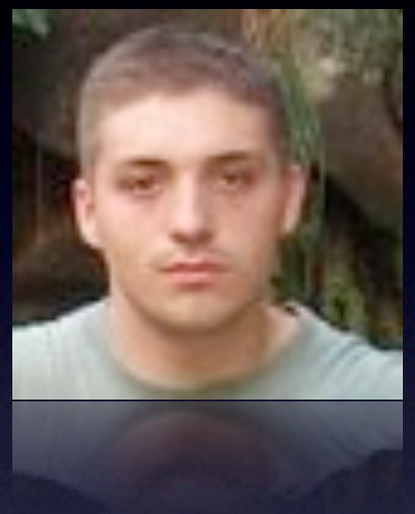


The Group

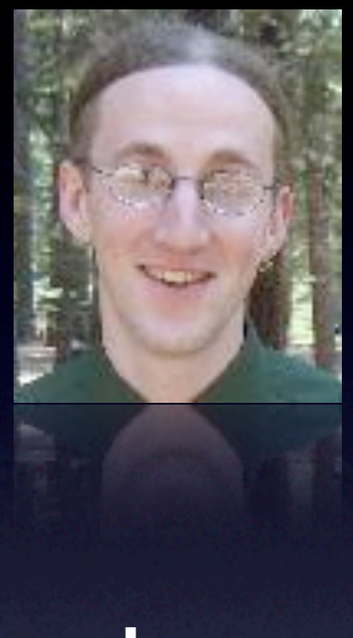
Graham



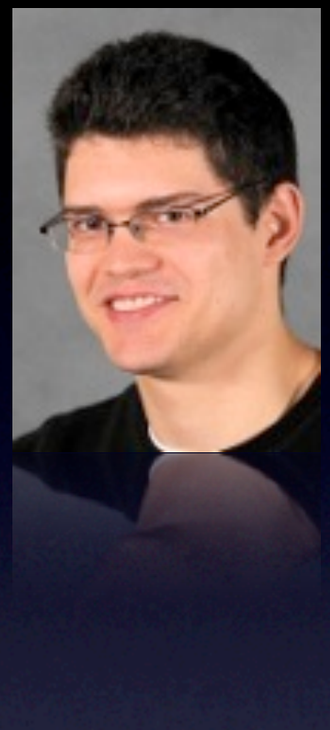
Piero



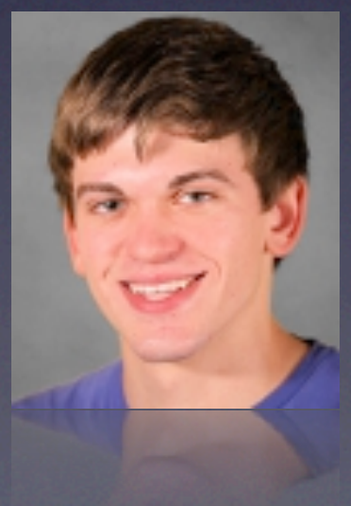
Brian



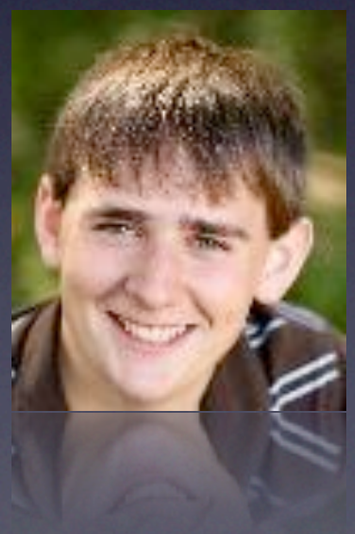
David



Brian

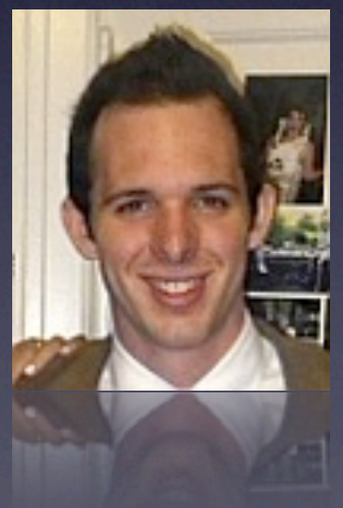


Daniel



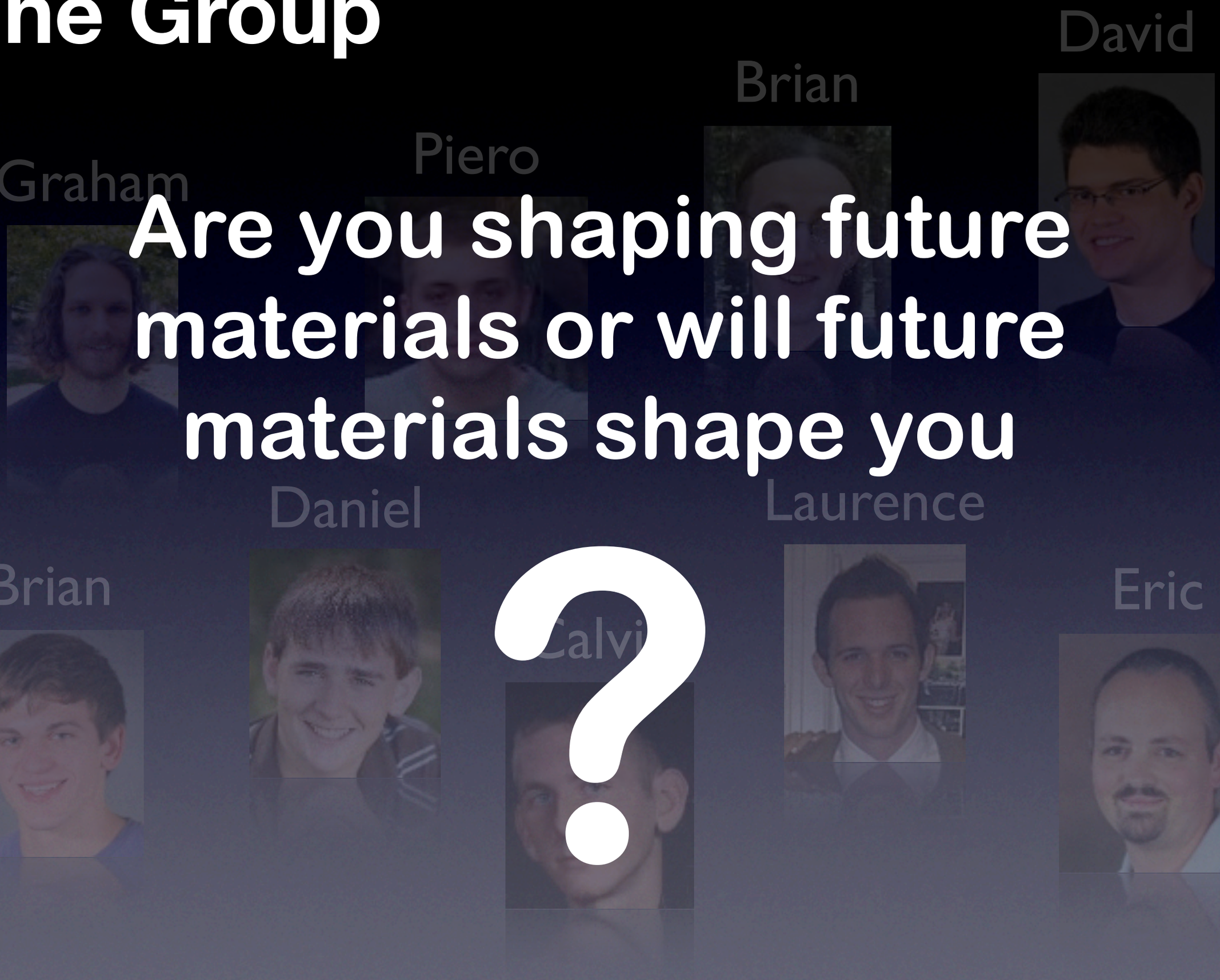
Calvin

Laurence



Eric

The Group


David
Brian
Piero
Graham
Are you shaping future materials or will future materials shape you
Daniel
Laurence
Brian
Calvi
Eric