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## Emergent magnetism in the titanium nitride

Titanium nitride (TiN) is a well-known technological material, a heat insulator of extreme hardness, used in high-performance coatings on other metals, as well as a non-toxic material for medical applications. It is also extensively used in the microelectronics industry. In none of these applications is it magnetic. However, in our first principal's density functional calculations we show that when TiN is strained by increasing the separation between atomic layers, resulting monolayers of TiN become magnetic. We show how this magnetism is activated or emergent as the layer separation gradually increases: at a critical separation, the magnetism turns on, and remains magnetic in a stable configuration. We also show how this may be experimentally realized, with the addition of, for example, Argon into TiN, to create TiN monolayers either in the bulk or at the surface. In addition, our analysis leads to an understanding of the source of magnetism in TiN monolayers, even in the midst of bulk TiN, and only separated from the bulk by monolayers of Ar. We present 3D illustrations of those wave functions and orbitals responsible for the magnetism and the effects of other layers on this magnetism. We also show some related model systems which show unexpected magnetic behavior.

### Biography

Barbara A Jones has been at IBM Almaden since 1989, working in a variety of areas from modeling magnetic recording devices to magnetic atoms on surfaces as studied by STM. She got her PhD from Cornell University in 1988, followed by a Postdoc at Harvard. She is on the Board of Physics and Astronomy of the National Academy of Sciences, an officer of the Physics Section of the AAAS, and an Honorary Member of the Aspen Center for Physics. She has been on the Editorial Boards of Physical Review X, Physical Review B, and Journal of Low-Temperature Physics.

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