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Electronic properties of Mn-decorated silicene and other 2D materials

Barbara A Jones

IBM Research – Almaden, USA

We first discuss silicene on hexagonal boron nitride, using first-principles calculations. Since hexagonal boron nitride is semiconducting, the interaction with silicene is weaker than for metallic substrates. Therefore, it is possible to open a 50meV band gap in the silicene. We further address the effect of Mn decoration by determining the onsite Hubbard interaction parameter, which turns out to differ significantly for decoration at the top and hollow sites. The induced magnetism in the system is analyzed in detail, and we compare and contrast with the behavior of other pairings of magnetic adatoms and 2D surfaces.

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.

bajones@us.ibm.com

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