# Atomic-layer resolved monitoring of Si(001) surface oxidation using RAS: A first-principles study

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The understanding of Si surface oxidation is both of great technological and fundamental interest. The microscopic mechanisms underlying the layer-by-layer oxidation are only partially explored [1]. Reflectance Anisotropy Spectroscopy (RAS) is an extremely useful technique allowing *in situ* observation of the oxidation process [2]. Inspired by recent experimental work we study the influence of layer-by-layer oxidation on the reflectance anisotropy spectra (RAS) of Si(001) numerically.
We present RA spectra for the energetically most favourable structures for different coverage. The calculations are performed within the gradient-corrected density functional theory (DFT-GGA) framework in conjunction with the projector-augmented wave (PAW) method. The optical spectra are calculated in the independent-particle approximation using all electron wave functions obtained from PAW method and corrected with respect to quasiparticle effects using scissors operators. Our results allow for the qualitative understanding of the experimentally observed RAS oscillation during layer-by-layer oxide growth. They are interpreted in terms of oxygen-induced change of the microscopic surface potential.

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# References

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