Probing the interaction between metals and oxide surfaces via EPR. The case of K atoms on alkaline-earth oxides.

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The study of the deposition of metal clusters and films on oxide surfaces is a subject attracting increasing interest [1,2]. The nature of the interaction between metal atoms and clusters and defect sites of the support material is particularly important in developing a molecular-level understanding of supported metal catalysts [3].

In this communication we report Electron Paramagnetic Resonance (EPR) and UV-Vis-NIR data relative to the adsorption of potassium metal atoms on the surface of MgO, CaO and SrO. A correlation between electron spin resonance and optical spectra for metal-electron species on the surface of ionic oxides is found. The very early stages of the metal-oxide interaction lead to the complete ionisation of the metal leading to an assembly of isolated fragments (M^+ and e^-) in which case the trapped electron forfeits any parentage in the electronic states of the gas-phase alkali atoms. Ab-initio quantum chemical modelling have shown that this reaction can occur on surface oxygen vacancies [4]. At slightly higher coverages situations also exist which are intermediate between the completely ionised and high atomic character limits. Here monomeric species retain the recognisable parentage of alkali atoms in the gas phase, but are subject to large perturbations arising from strong interaction with the substrate.

A close analogy is demonstrated between the optical and magnetic properties of alkali metal atoms on oxide surfaces and those of excited alkali metal atoms in the gaseous phase. Developing this analogy one can show how the techniques of electron paramagnetic resonance and optical spectroscopy can be used to give a quantitative measure of the metal-oxide interactions.

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