"Thermal stability of La2NiO4 and its Effect on Surface Reconstruction"

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La2NiO4 is a potential intermediate temperature solid oxide fuel cell (IT-SOFC) cathode material which belongs to the Ruddlesden-Popper (RP) structure series AO(ABO3)n. It offers a way to avoid Sr segregation and associated degradation, as Sr doping is not essential. While the bulk ionic conduction mechanisms are well studied, its surface structure and chemistry are still a matter of debate. Recent experimental work (both with and without dopants) reveals it has a La-terminated surface and a highly Ni deficient surface layer; this disagrees with earlier results from molecular simulations, and undermines the conventional explanation for the oxygen reduction process at the surface. In this work we evaluate the thermodynamic stability of La2NiO4 at IT-SOFC operation temperatures. We find that the decomposition of La2NiO4 to produce La2O3 and higher order RP phases is indeed thermodynamically favourable. In addition, the surface energies of La2NiO4 with different phases and terminations are evaluated using hybrid density functional theory method. Based on these results, a hypothesis for the formation mechanism of the La-terminated and Ni deficient surface based on partial decomposition and surface passivation is proposed and possible relevant process kinetics are evaluated.