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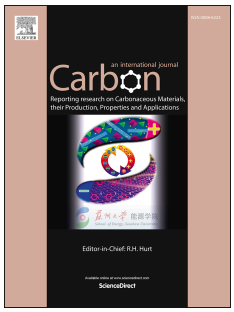

Two-dimensional siligraphenes as cathode catalysts for nonaqueous lithium-oxygen batteries

Huilong Dong, Yujin Ji, Tingjun Hou, Youyong Li

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Two-dimensional siligraphenes as cathode catalysts for nonaqueous lithium-oxygen batteries

Huilong Dong,* Yujin Ji, Tingjun Hou and Youyong Li*

Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, Jiangsu 215123, China.

Abstract

The nonaqueous lithium-oxygen ($Li-O_2$) battery is promising as a superior energy storage medium, whose practical applications are limited by the catalytic performance of cathode catalysts. Using density functional theory calculations, we systematically investigate the catalytic mechanism and catalytic performance of siligraphenes as cathode catalysts in nonaqueous $Li-O_2$ batteries. For the siligraphenes studied here, Li_2O is the final discharge product. Among them, the single-layered SiC (SL-SiC) exhibits potential as a suitable cathode catalyst due to the considerably low overpotential values during discharge and charge process. That is, 0.73 V for oxygen reduction reaction (ORR) and 1.87 V for oxygen evolution reaction (OER). The quantitative analysis indicates that the ORR overpotential on siligraphenes is linearly correlated with the ΔE_{ads} of the last added Li in Li_4O_2* (* denotes the adsorbed surface), while the OER overpotential is linearly correlated with the E_{ads} of LiO_2 on surface. Our investigations elucidate quantitative correlations between the catalytic performance of siligraphenes and the adsorption performance of Li-contained intermediates on them, which provides promising approach to develop metal-free cathode catalysts with high catalytic activity.

* Corresponding authors.

E-mail: huilong_dong@126.com, Tel: (86)-512-65882037 (H. Dong);

E-mail: yyli@suda.edu.cn, Tel: (86)-512-65882037 (Y. Li).