***Poster Abstract Template for NANO-SA-2023***

**“Intermetallic Copper-Based Electrode Catalyst with High Activity for C–H Oxidation and Cycloaddition of CO2 into Epoxides”**

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**Abstract:** *(times new roman, font size 12, word limit 200, and spacing 1.5)*

It has been proved that inorganic electrides are suitable hosts for integrating transition metals, which can serve as active sites and exhibit remarkable catalytic performance. In this work a reusable and recyclable (for more than 7 times) copper-based intermetallic electride catalyst (LaCu0.67Si1.33) fabricated, in which the Cu sites activated by anionic electrons with low-work function are uniformly dispersed in the lattice framework, shows vast potential for the selective C–H oxidation of industrially important hydrocarbons and cycloaddition of CO2 with epoxide. This leads to the production of value-added cyclic carbonates under mild reaction conditions. Importantly, the LaCu0.67Si1.33 catalyst enables much higher turnover frequencies for the C–H oxidation (up to 25 276 h–1) and cycloaddition of CO2 into epoxide (up to 800 000 h–1), thus exceeding most nonnoble as well as noble metal catalysts. Density functional theory investigations have revealed that the LaCu0.67Si1.33 catalyst is involved in the conversion of N-hydroxyphthalimide (NHPI) into the phthalimido-N-oxyl (PINO), which then triggers selective abstraction of an H atom from ethylbenzene for the generation of a radical susceptible to further oxygenation in the presence of O2.1

**Keywords:** *(Please provide 5 key words in alphabetical order separated with semicolons)*

C-H activation, Electride catalyst, Copper, Carbon dioxide, Cyclic carbonate

**References:** *(maximum 5, times new roman, font size 10, and spacing 1.15)*

1. Kadam, R. G.; Ye, T. N.; Zaoralová, D.; Medveď, M.; Sharma, P.; Lu, Y.; Zoppellaro, G.; Tomanec, O.; Otyepka, M.; Zbořil, R.; Hosono, H.; Gawande, M. B., Intermetallic Copper-Based Electride Catalyst with High Activity for C–H Oxidation and Cycloaddition of CO2 into Epoxides. *Small* **2022,** 2201712.

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