Pd single-atom heterogeneous catalyst on nitrogen doped carbon for sustainable Sonogashira cross-coupling

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Among the transition-metal catalyzed cross-coupling reactions, the Sonogashira-Hagihara reaction presents a cornerstone in today's synthetic chemists toolbox to access complex arylalkynes and enynes.[1] Attempts to replace homogeneous palladium catalysts with solid-supported, mostly nanoparticle-based counterparts have failed to compensate for inferior activity or severe metal leaching. Single-atom heterogeneous catalysts (SAHC) are promising approach to maximize the control over the palladium site, while displaying favorable metal-efficiency and facile recoverability.[2] Herein, we report Pd single-atoms supported on nitrogen doped carbon (**Fig. 1a**) as a sustainable catalyst for the Sonogashira cross-coupling. Advanced characterization techniques are used to relate structure properties with catalyst activity and stability. Although lower activity was observed compared to homogeneous benchmarks (**Fig. 1b**) the SAC stands out with its stable performance. A more holistic and process-centered assessment of the investigated catalysts is obtained through life cycle analysis (LCA), unveiling the sustainability of heterogeneously catalyzed Sonogashira coupling.

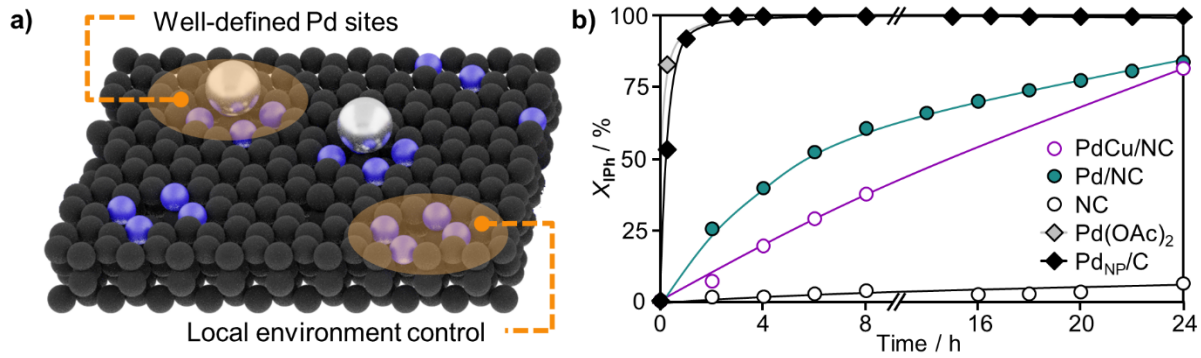

Fig. 1 a) Schematic representation of the surface of the Pd/NC catalyst (0.5wt% Pd loading). **b)** Catalytic performance of selected benchmark catalysts and Pd/NC.

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