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Title:	Unravelling charge-transfer in Pd to pyrrolic-N bond for superior electrocatalytic performance
Authors:	Sahoo, Lipipuspa (/jspui/browse?type=author&value=Sahoo%2C+Lipipuspa) Mondal, Sanjit (/jspui/browse?type=author&value=Mondal%2C+Sanjit) Gloskovskii, A. (/jspui/browse?type=author&value=Gloskovskii%2C+A.) Chutia, Arunabhiram (/jspui/browse?type=author&value=Chutia%2C+Arunabhiram) Gautam, Ujjal K. (/jspui/browse?type=author&value=Gautam%2C+Ujjal+K.)
Keywords:	charge-transfer pyrrolic-N
Issue Date:	2021
Publisher:	Publishing
Citation:	Journal of Materials Chemistry A, 9(17), 10966–10978.
Abstract:	Fuel-cells require large quantities of Pt for oxygen reduction reaction (ORR) to subvert the activity-loss during prolonged use. Pd can complement Pt in the near future by exhibiting a similar activity and stability in alkaline fuel-cells. Herein we show that by depositing Pd atom-by-atom on an N-doped reduced graphene oxide (NRGO), it is possible to create a strong bond between Pd and pyrrolic-fraction of the N-moieties. This bond further strengthens in the presence of an oxygen containing functional-group accompanied by a profound charge-transfer from the Pd 3d-orbitals to the 2p-orbitals of C, N and O, thereby lowering the Pd-3d binding-energy and the resulting Pd/NRGO exhibits a very high ORR activity ($E_{1/2} = 0.93$ V vs. RHE) and stability ($\Delta E_{1/2} = 0.013$ V after 15 000 cycles). Usually pyridinic-N is considered for imparting high-performance while N-doping creates nearly as many pyrrolic-N in graphene-substrates, the role of which is evidenced in this study.
Description:	Only IISERM authors are available in the record.
URI:	https://pubs.rsc.org/en/content/articlelanding/2021/TA/D0TA12618G (https://pubs.rsc.org/en/content/articlelanding/2021/TA/D0TA12618G) http://hdl.handle.net/123456789/4964 (http://hdl.handle.net/123456789/4964)
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