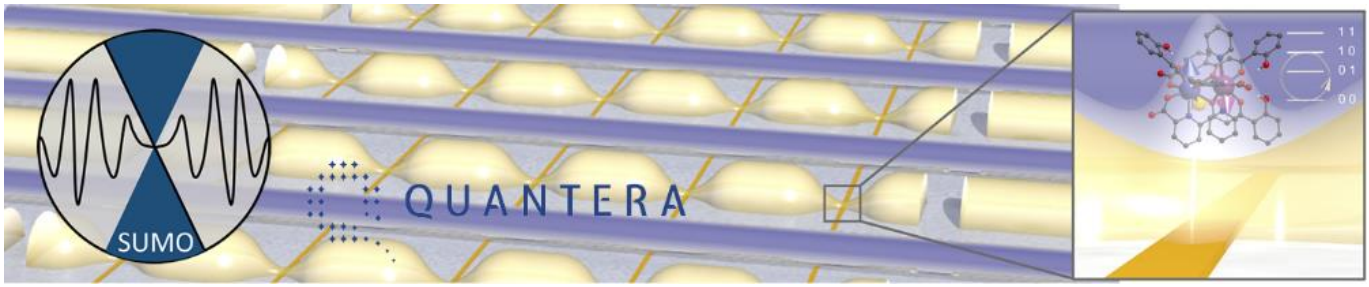

Open data management. Description of available data and metadata related to a publication	
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Date	2019/06/24
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Language	English
Dataset ID	SUMO_INSTMPR_Chiesa_PRB2019-1
List of data files available	Ni2_transport.mat
Methodology	This is a theoretical study based on ab-initio DFT calculations performed on the Jülich supercomputers JURECA and JUWELS.
Data processing and software needed	Calculations were done by employing NWChem quantum chemistry package (see website http://www.nwchem-sw.org/index.php/Main_Page). Data were processed and plotted using Matlab (version 2019a)
Access to the data	Contact Stefano Carretta at stefano.carretta@unipr.it