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Reaction mechanism of the oxidation of HCl over RuO_2(110) ARI SEITSONEN, Physikalisch-Chemisches Institut, University of Zurich, HERBERT OVER, Physikalisch-Chemisches Institut, Justus-Liebig-University, Giessen — Density functional theory (DFT) calculations reveal that the oxidation of HCl with oxygen producing Cl_2 and water proceeds on the chlorine-stabilized RuO_2(110) surface via a one-dimensional Langmuir-Hinshelwood mechanism [S Zweidinger *et al*, Journal of Phys. Chem. C **112**, 9966 (2008)]. The recombination of two adjacent chlorine atoms on the surface of the catalyst constitutes the rate-determining step in this novel Deacon-like process, having been recently introduced in the industrial chemistry by Sumimoto Chemical [K Iwanaga *et al*, Kagaku I, 1 (2004)]. The DFT results explain the high-resolution core level shift and temperature-programmed reaction experiments.

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