

*Pd(II)- LMOF for the sensing of molecular hydrogen in gas phase*Katherine Chulvi-Iborra¹, Werner Kraus¹, Knut Rurack¹, Franziska Emmerling¹¹FB 1.3 Strukturanalytik, Bundesanstalt Für Materialforschung Und prüfung (BAM), Berlin, Germany

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Current interest in hydrogen gas as an energy source is growing due to its attractive properties such as high chemical energy density and the fact that its combustion produces water as by-product, qualifying this gas as an appealing clean energy source. In particular, the use of molecular hydrogen in automotive applications such as the hydrogen internal combustion engine (HICE) or hydrogen fuel cells is an excellent clean alternative.

Despite these promising opportunities, hydrogen gas has a distinct disadvantage as an everyday energy medium, that is, it is highly flammable. Hydrogen processing apparatuses should therefore be constantly monitored so that leaks are immediately detected. The implementation of direct sensing systems for H₂(g) is thus a decisive factor for its application and acceptance as a clean energy source. Because the automotive market alone is already a mass market, these sensors do not only have to be reliable, robust and dimensionally small, but operation has to be simple and the device itself cost-effective. In addition, very low detection limits are a must as already escape of small quantities of H₂(g) is directly related to public health and safety. Besides electrochemical or semiconductor sensors, optical sensors are especially appealing because the equipment is usually simple and accessible, easily miniaturized and measurements can be performed in situ and in real time.

If one cannot rely for instance on metallic palladium as interacting matrix, a major challenge for optochemical hydrogen sensors is to find a suitable material that fulfils all the requirements mentioned above and undergoes a dedicated indication reaction with H₂(g). One such alternative can be Metal-Organic Frameworks (MOFs) which constitute a predefined, organized, mesoporous structure built up from metal ions and organic bridging ligands. With a myriad of building blocks being available, MOFs can be equipped with internal H₂ reception sites that shall allow for selective and sensitive indication. For instance, if Pd ions are implemented in such a way that they express open metal sites (OMS), these OMS shall possess a strong affinity for hydrogen. If light absorbing and emitting organic ligands are additionally chosen, luminescent MOFs (LMOFs) can result that are perfect candidates for optical sensors, as changes at the analyte reception site can be effectively transduced into a measurable signal.

In this contribution, we intended to discuss the development of a new luminescent sensor material for the detection of the highly flammable H₂(g). This sensor material is based on an LMOF assembled from Pd(II) and aromatic bridging ligands, the advent of hydrogen at the OMS in the LMOF producing distinct variations in the material's optical properties.

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