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for accelerating the development of clean and sustainable methods of producing hydrogen overall. The combination of experimental research and computational modeling gives a complete approach to understanding the catalytic activity of MgAl. This opens the door for the creation of water splitting devices that are both more effective and economically practical [1-6].

Experimental Section synthesis

A co-precipitation approach utilizing magnesium chloride ($MgCl_2$), aluminum chloride ($AlCl_3$), and sodium hydroxide ($NaOH$) may manufacture MgAl. In a beaker, equal amounts of $MgCl_2$ and $AlCl_3$ are combined. $NaOH$ is added dropwise while stirring. Monitoring the pH with a pH meter, $NaOH$ solution is added until it hits 8–10. After stirring for 1–24 hours, precipitation and particle growth occur.

The precipitate is filtered out after precipitation. Filtration removes undissolved solids. Washing the filter cake until the wash water's pH is neutral removes any remaining contaminants or Table 1 undesirable ions. Dried filter cake yields MgAl. Depending on product moisture and particle properties, drying may be done in an oven or at room temperature. The synthesis process depends on pH, temperature, and metal salt concentration. Co-precipitation works well at 50–70 °C and 8–10 pH. To create precipitates, metal salt concentrations like $MgCl_2$ and $AlCl_3$ must be kept between 0.1 and 0.5 M. Adjusting aging time, pH, and concentration controls MgAl product particle size and shape. MgAl with specific characteristics for catalysis, energy storage, and structural materials requires these synthesis considerations [5].

Computational details

In this investigation, the characteristics of MgAl were analyzed using a DFT calculation that was carried out in Material Studio. During the course of the investigation, the CASTEP module—which is well-known for its applicability in DFT calculations—was used. The typical cell of MgAl had its lattice parameters adjusted such that $a = 4.99$, $b = 4.99$, $c = 5.50$, $\alpha = 90.00^\circ$, $\beta = 90.00^\circ$, and $\gamma = 120.00^\circ$, with a volume that ended up being 118.56 Å³. The following is a description of the atomic locations found inside the unit cell: the magnesium atom inhabited the 2c Wyckoff position with the coordinates (2/3, 1/3, 3/4), and the aluminum atom held the 2d Wyckoff position with the coordinates (2/3, 1/3, 1/4). It was found that the crystal structure was hexagonal,

stages (R2), (R3), (R4), and (R5), respectively. According to equation (6), the OER performance of the MgAl catalyst is going to be superior in proportion to the overpotential's decrease [1].

Result and Discussion

XRD

In the XRD graph that I drew, which displays the intensity of X-ray diffraction as a function of the 2θ angle, I saw numerous peaks that give insights into the crystalline qualities of my catalyst material in relation to water splitting. These features are important because they allow the material to perform its job as a catalyst.

The initial peak, which was also the most conspicuous, occurred at a value of $2\theta = 20.5$ and had an intensity of 941. This peak reveals that my catalyst material has a large crystallographic plane that plays an important role in the process of water splitting. It seems to imply

has an effect on the electronic structure of the catalyst, which in turn has an effect on its capacity to interact with water molecules and to assist the essential redox processes. A high charge density may result in greater contact between the catalyst and the reactant species, which in turn promotes efficient charge transfer and makes the process of water splitting easier [6]. The charge density may also have an effect on the stability and reactivity of surface sites on the catalyst. The charge density determines the availability of active sites for water adsorption and the following reaction steps. These active sites must be easily accessible. A sufficient number of active sites and their correct distribution may be ensured by achieving the optimal charge density, which in turn boosts the catalyst's overall efficiency. In addition, the charge density may have an effect on the electrochemical potential as well as the overpotential of the catalyst when it is in use in the process of water splitting. The charge density that exists at the interface between the electrolyte and the catalyst has an effect on the kinetics of charge transfer as well as the activation energy that is required for the different reaction steps. An appropriate charge density may help to limit energy losses and lower the needed overpotential for water splitting, enhancing the catalyst's overall efficiency.

Results

The OER, or oxygen evolution reaction, is a process that is involved in the process of water splitting. This reaction consists of a succession of four elementary electron phases. These stages are responsible for the transformation of molecules of water and intermediates into oxygen gas (O₂) and protons (H⁺). The kind of catalyst used has a significant impact on how well the process of splitting water works. Due to the fact that it has the capability of splitting water, the MgAl catalyst is of special importance in this setting. On the other hand, particular information on its performance and whether or not it is suitable for this procedure has not been supplied. In order to investigate the crystalline characteristics of the MgAl catalyst, an XRD examination was carried out. Even though the peaks were characterized in terms of their locations and intensities, it was not possible to establish a clear link between those characteristics and the catalyst's capacity for water splitting. It was discovered that the charge density of the MgAl catalyst was a significant factor in determining the water splitting catalytic activity of the catalyst. This parameter has an effect on the electronic structure of the catalyst as well as its stability and reactivity. It plays a part in enabling interactions with water molecules, affecting the availability of active sites, and having an influence on the overpotential that is necessary for water splitting. In addition, a phase diagram was shown, which depicted the formation energies and percentages of the various phases that exist inside the Mg-Al system while the temperature was 0 degrees Celsius. Pure Mg, Mg₁₇Al₁₂, MgAl₂, and pure Al were present throughout the stages. Even though the phase diagram shows information about how stable these phases are and what they are made of, the direct effect that these phases have on how well the MgAl catalyst splits water was not talked about in the last section. In a nutshell, the content of our discussion has shed light on numerous parts of the water splitting process as well as the MgAl catalyst. However, in order to draw more certain conclusions regarding the effectiveness of the MgAl catalyst in driving this essential reaction, further information and study specifically pertaining to the performance of the MgAl catalyst in water splitting are required [5][1].

Discussion

Findings that have been described give an initial grasp of the elements that influence water splitting as well as the potential of the MgAl catalyst. The XRD graph was analyzed, and the results showed

the existence of different peaks, which indicated the presence of crystalline phases inside the catalyst. However, further research is required to determine whether or not there is a direct connection between these phases and the efficiency of the catalyst in water splitting [2]. It was discovered that the charge density of the MgAl catalyst was a critical parameter impacting the catalytic activity of the catalyst. A greater charge density may improve interactions with water molecules and facilitate effective charge transfer, which may result in an increase in the catalyst's water-splitting activity. Nevertheless, further in-depth research is necessary in order to completely clarify the connection between charge density and catalyst performance [1]. The phase diagram reveals information on the stability of several phases in the Mg-Al system as well as the makeup of those phases. Some phases, such as Mg₁₇Al₁₂ and MgAl₂, show that catalytic activity might be possible. However, more research needs to be done to find out how directly these phases affect how well the MgAl catalyst works to split water [2].

Future Recommendation

Complete grasp of the structure and components that make up the catalyst. Methods like X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM) may provide very helpful insights into the crystallographic characteristics, active sites, and surface chemistry of a catalyst. With this new information, we will be able to get a more in-depth understanding of the behavior of the catalyst throughout the process of water splitting. In addition, performing electrochemical tests is very necessary in order to evaluate the catalytic activity and performance of the MgAl catalyst under the appropriate circumstances. Methods such as cyclic voltammetry and chronoamperometry are able to offer quantitative data on the electrochemical behavior of the catalyst in addition to the reaction kinetics and stability of the catalyst. The results of these trials will provide vital insights into the efficiency of the catalyst and its potential for use in water splitting applications on a broad scale [3]. Computational modeling may be a very helpful tool in predicting and comprehending the behavior of the catalyst, especially when it is used in conjunction with experimental research. Calculations based on density functional theory (DFT) have the potential to shed light on the electronic structure, energetics, and reaction processes involved in the process of water splitting on the MgAl catalyst. This kind of modeling may be used to direct the design of innovative catalyst materials and give more in-depth knowledge of the activities that are occurring under the surface. Catalyst design and synthesis may be improved by drawing upon the insights obtained through characterization, experimental testing, and computational modeling. In order to improve the catalytic efficiency and stability of the catalyst, this step may entail altering the composition of the catalyst, including dopants in the catalyst, or designing the catalyst's shape. It is possible to build catalysts for the process of water splitting that have enhanced activity, selectivity, and durability via iterative design and synthesis.

Conclusion

It is essential to conduct long-term stability experiments in order to properly assess the performance of the catalyst over a prolonged period of time. In order to assure the practical feasibility and long-term sustainability of the MgAl catalyst in water splitting applications, conducting research into aspects such as catalyst deterioration, corrosion, and fouling is necessary [2]. If these future suggestions are followed, one will be able to gain more in-depth knowledge of the MgAl catalyst's potential for water splitting. This information will pave the way for the development of catalyst materials that are efficient, stable,

