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1. Experimental Section

Ethane bromide (99.0%) was purchased from TCI. Tetrahydrofuran (99.5%) was purchased from Amethyst and refluxed for over 24 hours before reaction.

The reagents were transferred by syringes. The reaction was carried out in a 10ml Schlenk tube. The magnesium turnings (1065.5 mg) and copper mesh (4729.0 mg) was folded to fit into the Schlenk tube, and connected to the multimeter (measure range: 0-2mA, precision: $\pm 1 \mu\text{A}$) with iron wire. The vessel was purged 3 times with N_2 ; 10 ml of THF was injected into the vessel, 0.1ml EtBr was subsequently injected. Both copper mesh and magnesium were reacted without any pre-treatment, no stirring was applied during the reaction process. The electronic current was measured continuously and recorded every 20 seconds.

After 3 hours of reaction, the magnesium turning and copper mesh were washed using ethanol and dried. The weight of copper was essentially unchanged after the reaction (4728.9 mg). 732.5 mg of magnesium was recovered, the weight loss of magnesium was used to estimate the reaction amount. For comparison, no current was observed using copper mesh and zinc sheet as electrodes. Also, no current was observed when the two electrodes were put into two separate reaction tubes.

2. Computational details

2.1. PES scan with customized optimizer

The PES scanings were done at lower theoretical level, with gamma point only k-point mesh and a cutoff energy of 300eV, the wavefunctions were converged to 1×10^{-4} eV, and the max force acting on atoms less than 0.05 eV/Å.

The constraint was defined as following, which treats the C-Cl bond as a rigid bond with fixed bond orientation and length. The bond was also constrained to one of the hcp sites in the x-direction (perpendicular to the rotaion plane) to avoid hopping between adjacent sites.

```
import numpy as np

class myBondFix:
    def __init__(self, r, theta):
        self.theta = theta
        self.r = r

    def adjust_positions(self, atoms, newpositions):
        newpositions = fix_bond(atoms, self.r, self.theta, newpositions)

    def adjust_forces(self, atoms, forces):
        cl = np.where(atoms.numbers == 17)[0]
        c_index = np.where(atoms.numbers == 6)[0]
        alpha_c = c_index[np.argmin(atoms.get_distances(c_index, cl))]
        pair = [cl, alpha_c]
        forces[pair, :] = forces[pair, :] + forces[pair[:-1], :]
        forces[pair, 0] = 0

def fix_bond(atoms, i, theta, pos):
    cl = np.where(atoms.numbers == 17)[0]
    h_index = np.where(atoms.numbers == 1)[0]
    c_index = np.where(atoms.numbers == 6)[0]
    index_r = list(h_index) + list(c_index)
    alpha_c = c_index[np.argmin(atoms.get_distances(c_index, cl))]
    pos[cl, 0] = 3.1414999999999999
    a = pos[alpha_c, :] - pos[cl, :]
    z = [0, 0, 1]
    v = -np.cross(a/np.linalg.norm(a), z)
    c = np.dot(a/np.linalg.norm(a), z)
    s = np.linalg.norm(v)
    v_x = np.transpose(v)
    v_x = [[0, -v[2], v[1]],
           [v[2], 0, -v[0]],
           [-v[1], v[0], 0]]
    v_x = np.array(v_x)
    if s == 0:
        rotate_to_z = np.eye(3)
    else:
        rotate_to_z = np.eye(3) + v_x + np.dot(v_x, v_x) * (1-c)/s**2

    rotate_to_theta = [[1, 0, 0],
                      [0, np.cos(theta), np.sin(theta)],
                      [0, -np.sin(theta), np.cos(theta)]]

    rel_pos = pos[index_r, :] - pos[cl, :]
    rel_pos = np.dot(rel_pos, rotate_to_z)
    rel_pos[:, 2] += (i - np.linalg.norm(pos[alpha_c, :] - pos[cl, :]))
    rel_pos = np.dot(rel_pos, rotate_to_theta)
    pos[index_r, :] = pos[cl, :] + rel_pos
    return pos
```

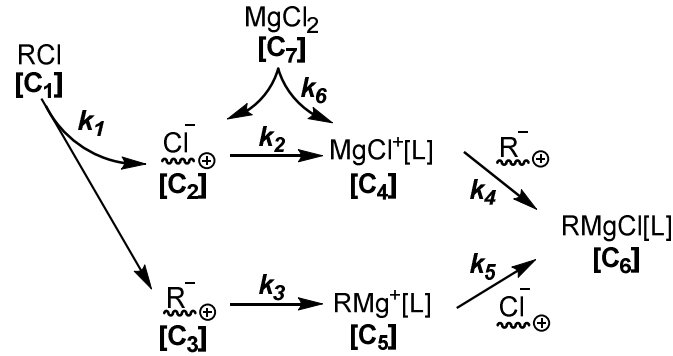
2.2. Wave function convergence

Wave function for structures containing cations are hard to converge with default settings due to bad initial guess. We managed to converge these structures by feeding converged wave function of adsorbed structures to desorbed structures.

2.3. Kinetic Model

The detailed kinetic model is shown in Figure S2. Pit corrosion behavior is modeled by a spherical single pit on a surface, the cationic desorption only happens in the pit region while dissociation can occur in any region. The pit area was set to a very small value (1×10^{-30} , dimensionless) at the beginning and grows as desorption proceeds. The total surface area were choosen ($A_0=5$, dimensionless) so that the final pit area($A_{pit} \approx 2$, dimensionless) is comparable to the total surface area, changing the total surface area didn't influence the kinetic feature significantly. The model is admittedly very simplified: the same surface concentration was used for kinetics without considering the adsorption/desorption of each species; and the kinetic parameters were cauculated using uncorrected electronic energies. Therefore, the model could only demonstrate the activation process qualitatively.

For the simulation without $MgCl_2$, C_1 was set to 1 (dimensionless); other concentrations were set to zero. For the simulation with $MgCl_2$, C_1 and C_7 were set to 1; other concentrations were set to zero.



$$\frac{dC_1}{dt} = A_{sum} C_1 k_1 \quad (Eq\ 3-1)$$

$$\frac{dC_2}{dt} = A_{sum} C_1 k_1 - A_{pit} C_2 k_2 - A_{sum} C_2 C_5 k_5 \quad (Eq\ 3-2)$$

$$\frac{dC_3}{dt} = A_{sum} C_1 k_1 - A_{pit} C_3 k_3 - A_{sum} C_3 C_4 k_4 \quad (Eq\ 3-3)$$

$$\frac{dC_4}{dt} = A_{pit} C_2 k_2 - A_{sum} C_3 C_4 k_5 \quad (Eq\ 3-4)$$

$$\frac{dC_5}{dt} = A_{pit} C_3 k_3 - A_{sum} C_2 C_5 k_5 \quad (Eq\ 3-5)$$

$$\frac{dC_6}{dt} = A_{sum} C_2 C_5 k_5 + A_{sum} C_3 C_4 k_4 \quad (Eq\ 3-6)$$

$$R_{pit} = \left(\frac{3C_4}{2\pi C_{1,0}} \right)^{1/3} \quad (Eq\ 3-7)$$

$$A_{pit} = 2\pi R_{pit}^2 \quad (Eq\ 3-8)$$

$$A_{sum} = 6 + A_{pit} - \pi R_{pit}^2 \quad (Eq\ 3-9)$$

$$k_i = e^{-\frac{E_a}{RT}}, i = 1, 2, 3, 4, 5 \quad (Eq\ 3-10)$$

$$E_{a,4} = E_{a,5} = E_{a,6} = 0 \quad (Eq\ 3-11)$$

Figure S1: Simplified kinetic model of GRF.

3. Benchmarking

Important parameters were benchmarked to ensure the convergence of our results. Most results showed our settings sufficient to converge the reaction energies and barrier energies. Though some of the energies still suffer an error of around 1 kcal mol⁻¹ with our 3x3x1 k-points mesh, our conclusion is not affected, and our PES scan under gamma point can be justified since only general selectivity pattern is interested.

3.1. K-point mesh

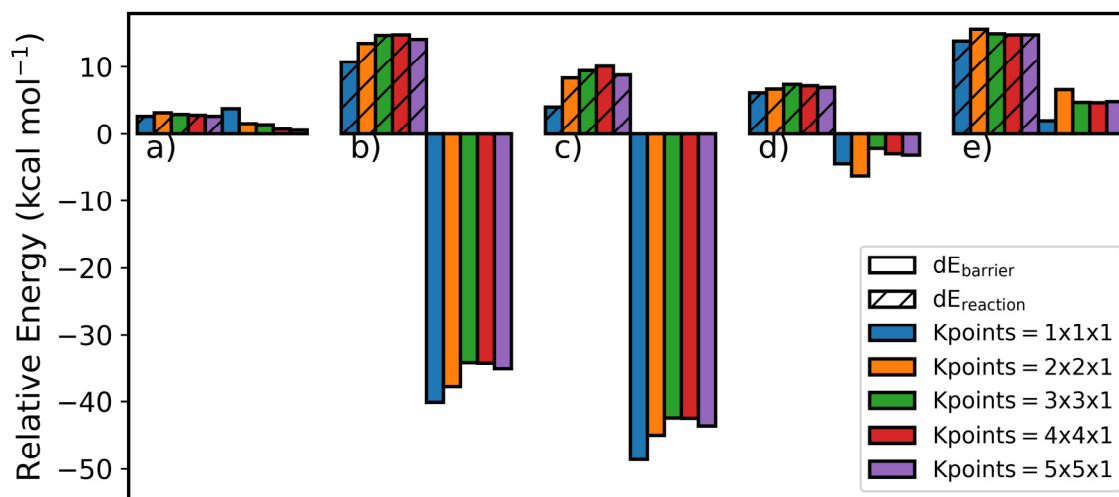


Figure S2: Reaction barriers and energies with different K-point mesh. For a) diffusion of Cl from Methyl group, b) horizontal dissociation of phenyl chloride, c) ionic dissociation of vinyl chloride, d) vertical dissociation of methyl chloride, e) desorption of MgVi⁺.

3.2. Cut-off energy

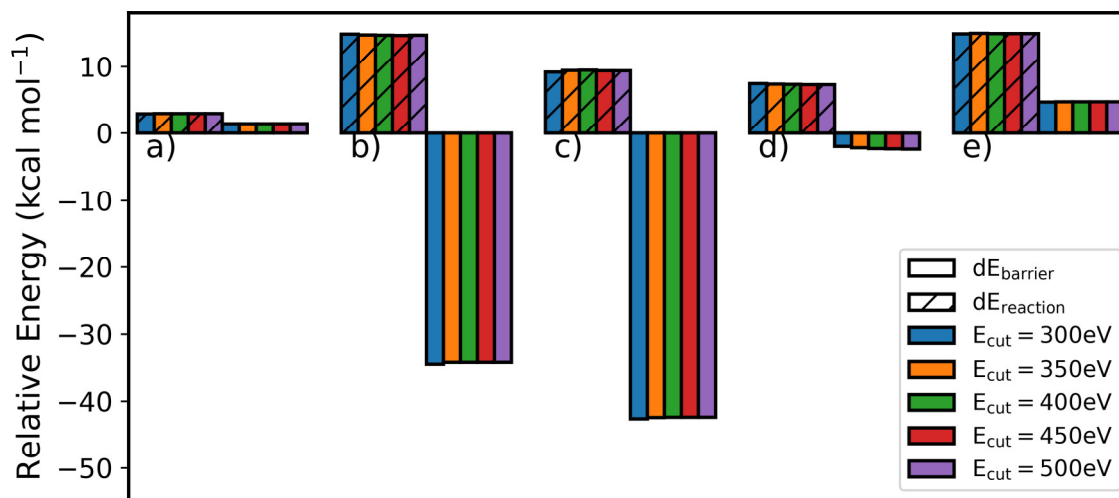


Figure S3: Reaction barriers and energies with different cutoff energy. For a) diffusion of Cl from Methyl group, b) horizontal dissociation of phenyl chloride, c) ionic dissociation of vinyl chloride, d) vertical dissociation of methyl chloride, e) desorption of MgVi⁺.

3.3. Smearing

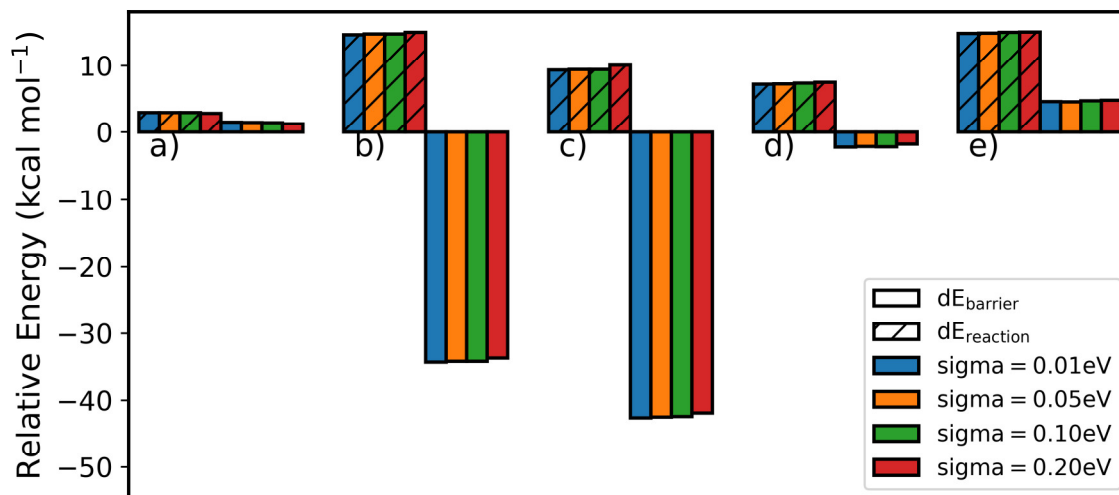


Figure S4: Reaction barriers and energies with different smearing (sigma value). For a) diffusion of Cl from Methyl group, b) horizontal dissociation of phenyl chloride, c) ionic dissociation of vinyl chloride, d) vertical dissociation of methyl chloride, e) desorption of MgVi⁺.

3.4. Vacuum layer size

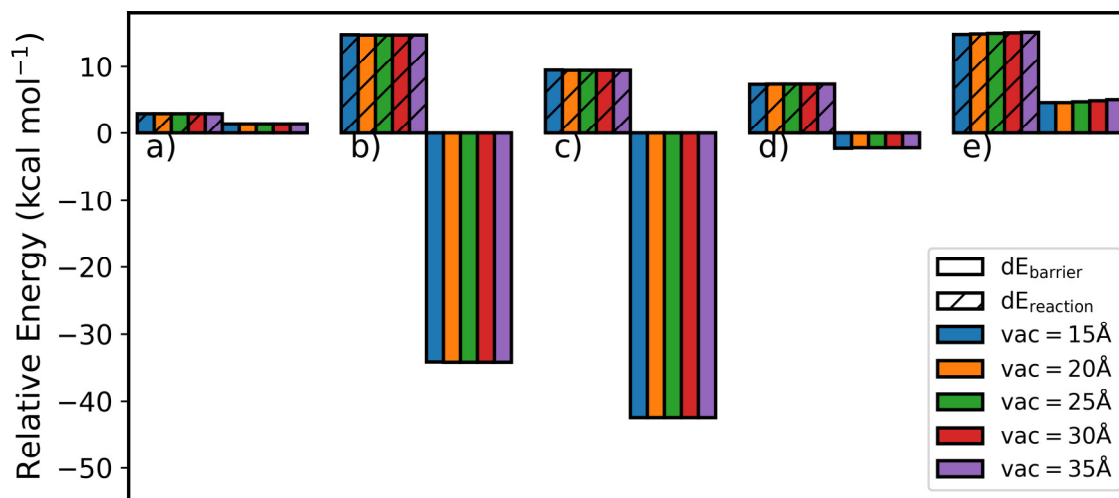


Figure S5: Reaction barriers and energies with different vacuum layer. For a) diffusion of Cl from Methyl group, b) horizontal dissociation of phenyl chloride, c) ionic dissociation of vinyl chloride, d) vertical dissociation of methyl chloride, e) desorption of MgVi⁺.

3.5. Entropy effect

We investigated the contribution of zero-point energy and the free energy correction at 300K, with all degrees of freedom treated harmonically. The contribution to a selected lists the reaction barriers and reaction energy of the key element steps discussed in the article are shown in Table S1.

Table S1: Relative electronic energy and Gibbs free energy of the transition state and product for selected reaction steps (in kcal mol⁻¹).

	$\Delta E^\ddagger$	$\Delta G^\ddagger$	ΔE	ΔG
Horizontal dissociation of MeCl	10.3	7.5	-40.5	-40.1
Vertical dissociation of MeCl	9.7	6.3	0.2	-6.1
Horizontal dissociation of PhCl	14.7	12.2	-34.1	-35.3
Vertical dissociation of PhCl	18.8	15.6	14.5	9.9
Diffusion of Cl atom from methyl group	2.9	3.3	1.4	0.6
Desorption of MeMg ⁺ cation	13.8	13.9	-0.3	-0.9

Generally, the Gibbs free energy barrier or free energy change is lower (by about 2-5 kcal mol⁻¹) for dissociation steps, where new fragment (radical or surface anion) is formed. The relative trend of reaction energy and barriers remains unchanged. Thus, our proposed mechanism is not influenced by the entropy effect.

As in our current version of VASP, the hessian matrix can only be evaluated numerically, calculating the Gibbs free energy for all the structures would take enormous amount of time. Therefore, we chose to use electronic energies for the discussion in the main article.

4. Supplemental data

4.1. Partial charge and DOS plot for vinyl and phenyl chloride

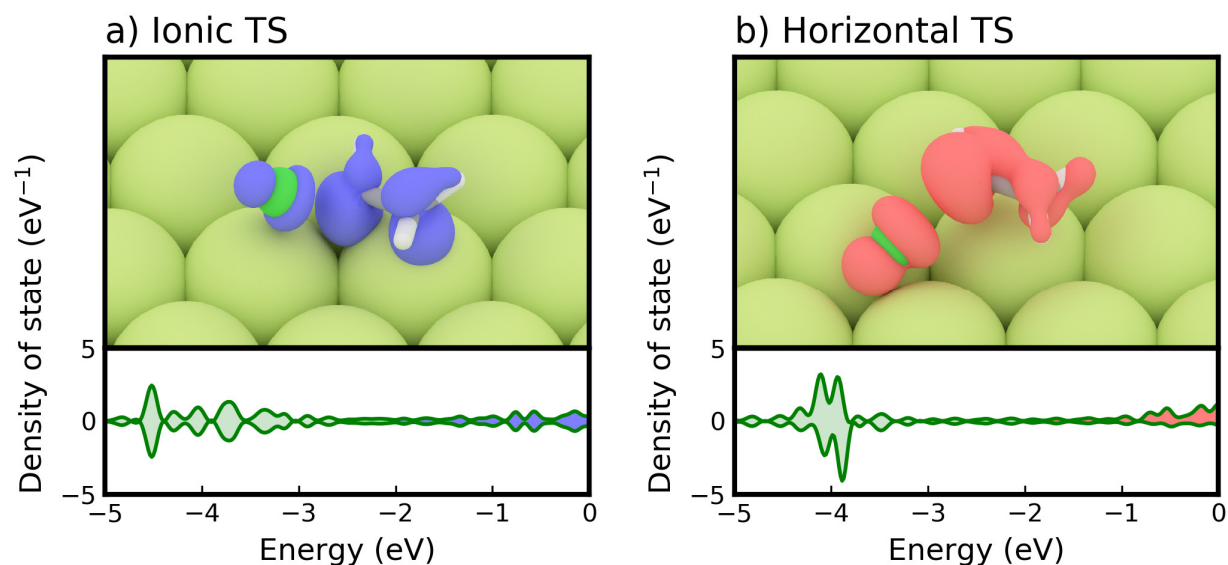


Figure S6: Partial charge density isosurface (0.06 electrons $\text{\AA}^{-3}$) and decomposed DOS (sum of C, H, Cl) plot of a) ionic and b) horizontal dissociation transition state for VinCl. In both cases, integration for DOS below -2eV gives 18 electrons, which is equal to the valence electrons of VinCl. The shown partial charge density therefore corresponds to the electrons transferred from the surface to VinCl molecule, whose integration equals to 2 for ionic TS and 1 for horizontal TS, respectively.

4.2. Diffusion pathways of surface species

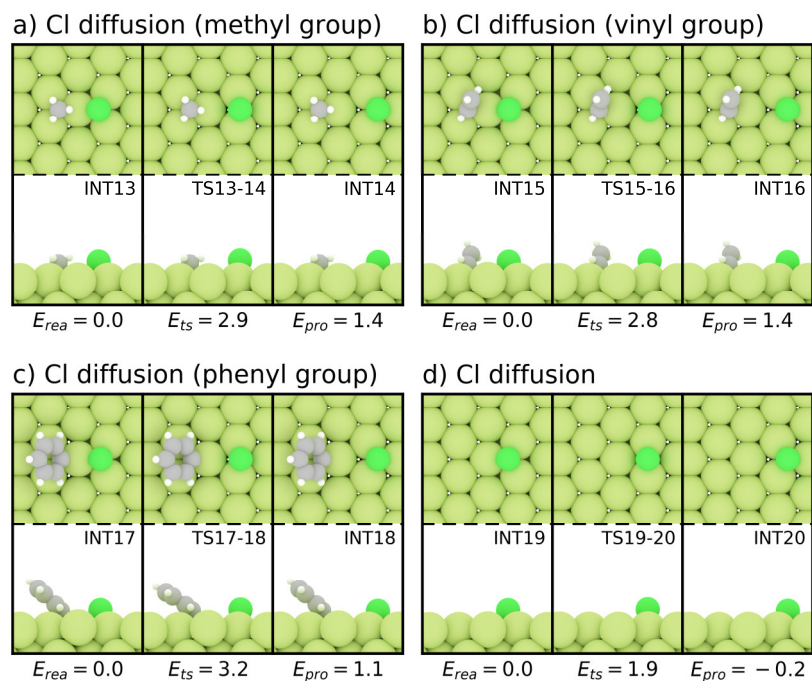


Figure S7: Reaction pathways of Cl diffusion from different anions (or alone) on Mg surface. Energies (kcal mol^{-1}) are relative to reactant species.

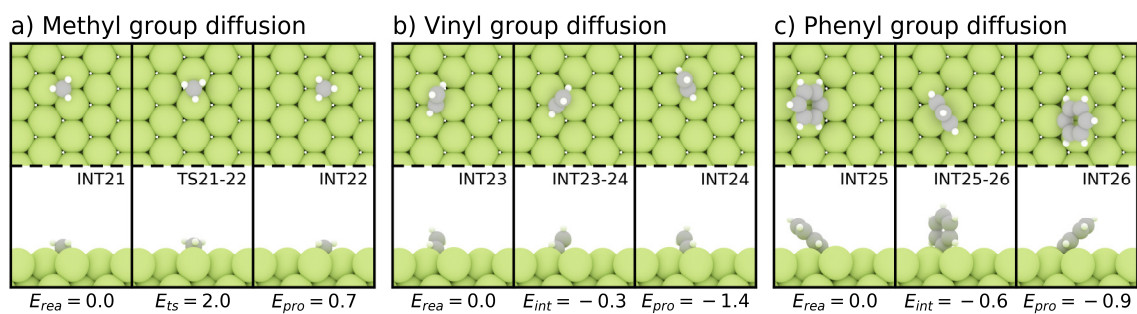


Figure S8: Reaction pathways of anion diffusions on Mg surface. Energies (kcal mol^{-1}) are to reactant species. No transition states were found for vinyl and phenyl group, probably due to too small barrier energy.

4.3. Desorption pathways of surface species

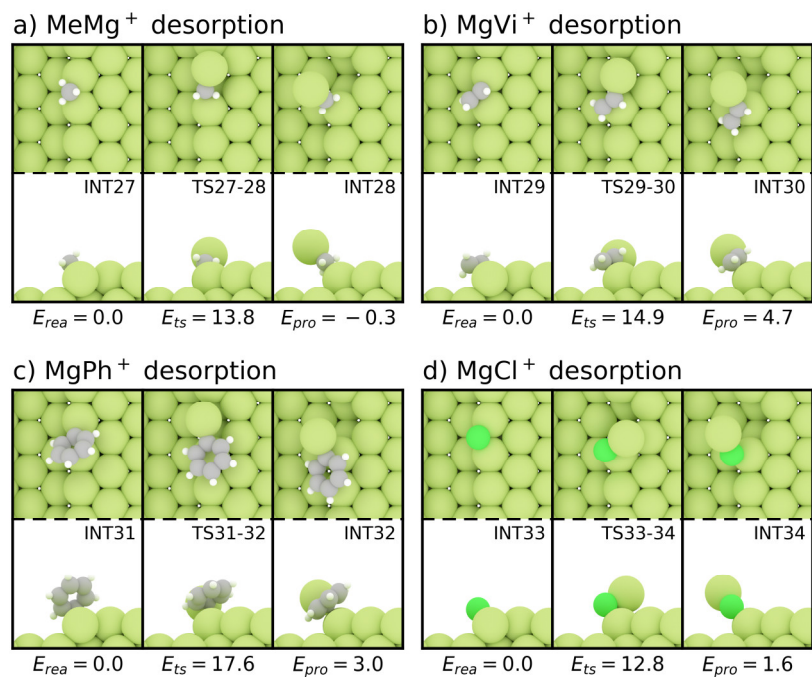


Figure S9: Reaction pathways of cation desorptions from Mg step site. Energies (kcal mol⁻¹) are relative to reactant species.

4.4. Formation pathways

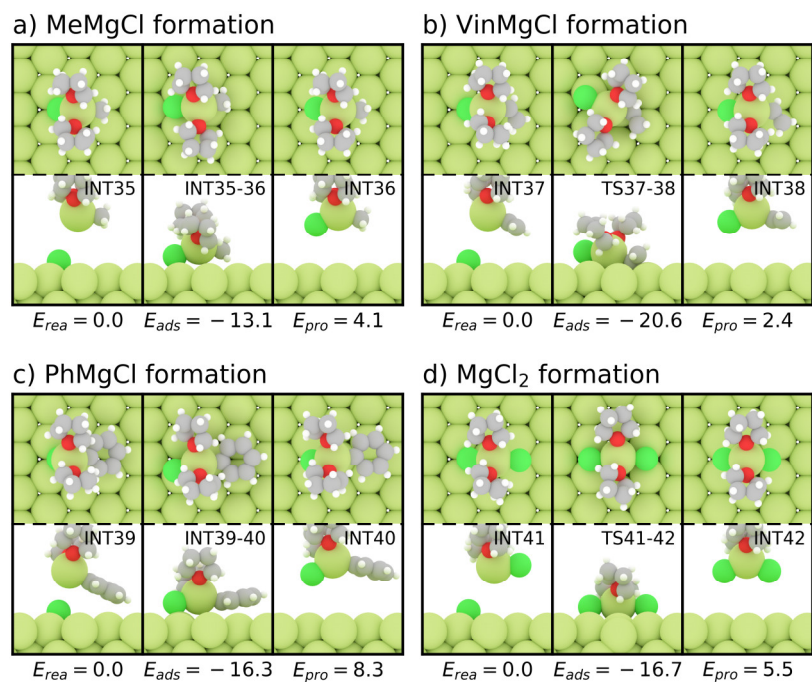


Figure S10: Reaction pathways of for the formation step. Energies (kcal mol⁻¹) are relative to cationic species.

4.5. Flipping of surface benzonorbornadienyl group

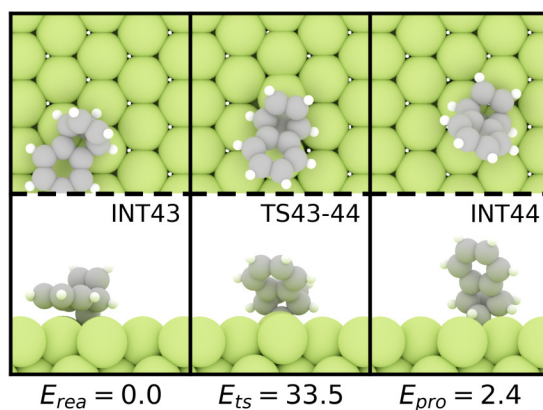


Figure S11: Reaction pathway for flipping of surface benzonorbornadienyl group. Energies (kcal mol⁻¹) are relative energies compared to reactant species.

4.6. Desorption energy plot for different species

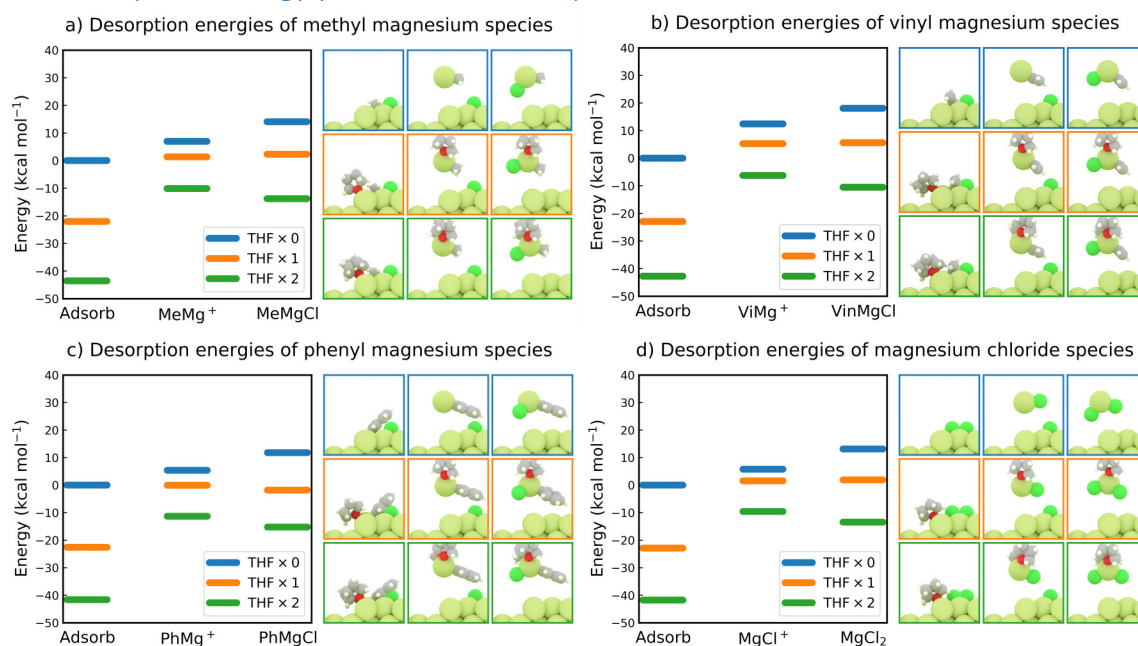


Figure S12: Desorption energy graph of magnesium with different organic group and solvent coordination. Energies (kcal mol⁻¹) are relative to adsorption structure and free THF molecules.

4.7. Influence solvents on reaction pathways.

To investigate the influence of different solvents on the reaction pathways, we revisited selected pathways with diethyl ether (DEE): another commonly used solvent for Grignard reagent formation, and compared them to the results obtained in tetrahydro furan (THF).

For most of the elementary steps we discussed, different solvents do not affect the reaction barriers and enthalpies significantly (Table S2). However, the cation desorption pathway (Figure 6 in manuscript) is not feasible with the diethyl ether solvent.

Table S2: Relative energy with DEE($\epsilon=4.33$) and THF($\epsilon=7.58$) of the transition state and product for selected reaction steps (in kcal mol⁻¹).

	$\Delta E_{THF}^\ddagger$	$\Delta E_{DEE}^\ddagger$	ΔE_{THF}	ΔE_{DEE}
Horizontal dissociation of MeCl	10.3	10.2	-40.5	-40.6
Vertical dissociation of MeCl	9.7	9.6	0.2	0.2
Horizontal dissociation of PhCl	14.7	14.7	-34.1	-34.1
Vertical dissociation of PhCl	18.8	19.0	14.5	14.9
Diffusion of Cl atom from methyl group	2.9	3.0	1.4	1.4
Desorption of MeMg ⁺ cation	13.8	-	-0.3	-

As the energies of MeMgCl desorption intermediates in diethyl ether shows, the desorption of the bare MeMg⁺ cation becomes highly unlikely in DEE (Figure S13). This is mainly due to the strong charge separation in the cation structures: ions are generally more stable in polar solvents. However, the cation intermediate is still stabilized with explicit solvent coordination. The desorption energy of the cation is lowered to -2.7 kcal mol⁻¹ with one DEE coordination. That is, although the bare cation desorption in less polar solvents like DEE is not feasible, cation desorption with concerted solvent coordination is still possible. With that said, the evaluation of such a concerted desorption/coordination pathway requires the inclusion of both surface-adsorbed solvents and solvent-phase solvents in the super cell, which is too expensive at the current level of theory.

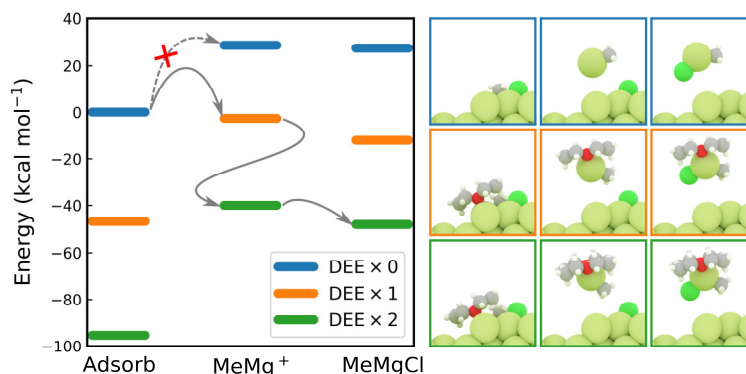


Figure S13: Desorption energy graph of magnesium with methyl group and solvent coordination. Energies (kcal mol⁻¹) are relative to adsorption structure and free DEE molecules. Possible reaction pathway is indicated with grey arrows.


```
-1.5631451309984357 10.1402757633512479 7.6762335876907573 T T T
-3.1414999999999251 10.882475223999647 0.0000000000000000 F F F
-3.1414999214624828 12.6962210493229701 2.5394499999999609 F F F
-3.1344662250446089 10.8780924096109484 5.0642482794223715 F F F
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6.2829999999999666 0.0000000000000000 0.0000000000000000 F F F
6.2830000785375386 1.8137458253230103 2.5394499999999609 F F F
6.2926955993181837 0.0148693470971711 5.0925241507835723 T T T
4.7122499999999539 2.7206188060000391 0.0000000000000000 F F F
4.7122500785375161 4.5343646313230481 2.5394499999999609 F F F
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3.1414999999999877 5.4412376119999823 0.0000000000000000 F F F
3.1415000785375486 7.2549834373229913 2.5394499999999609 F F F
3.1472201723013526 5.4272922609391792 5.1623449022804175 T T T
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1.5707500785375297 9.9756022432320278 2.5394499999999609 F F F
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-0.0000000000000000 10.882475223999647 0.0000000000000000 F F F
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POSCAR for INT30 ### Mg C H 1.0000000000000000 15.7074999999999996 0.0000000000000000 0.0000000000000000 -7.8537499999999998 13.6030940000000005 0.0000000000000000 0.0000000000000000 0.0000000000000000 0.0000000000000000 35.1578000000000017 90 2 3 Selective dynamics Cartesian 0.0000000000000000 0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F 0.000000785374505 1.8137458213230107 2.5394500034680880 F F F -0.0048618816846212 0.0414198470340396 5.0833218368406482 T T T -1.5707500000000219 2.7206188000000382 0.0000000000000000 F F F -1.5707499214625715 4.5343646213230482 2.5394500034680880 F F F -1.5757405569535838 2.7229892807107419 5.171724363961895 T T T -3.1414999999999886 5.4412375999999805 0.0000000000000000 F F F -3.1414999214624264 7.2549834213229909 2.5394500034680880 F F F -3.1421571777346196 5.4392866354184495 5.1891662603721525 T T T -3.1616876416551527 7.523331189938421 7.5580717697010609 T T T -4.7122500000000107 8.1618564000000191 0.0000000000000000 F F F -4.7122499214624476 9.9756022213230295 2.5394500034680880 F F F -4.7068281172849709 8.1839390967073058 4.99577736253939 T T T -4.7202373419835748 10.1719880810441558 7.6896157907919358 T T T -6.2829999999999773 10.8824751999999609 0.0000000000000000 F F F -6.2829999214624710 12.6962210213230691 2.5394500034680880 F F F 9.4115099124421420 10.8877467104148096 5.0766396317331282 T T T -6.3011853637745583 12.8177412614511930 7.577757896177641 T T T 3.1415000000000437 0.0000000000000000 0.0000000000000000 F F F 3.1415000785374940 1.8137458213230107 2.5394500034680880 F F F 3.1340835362877852 0.031244957177225 5.086273354808092 T T T 1.5707500000000219 2.7206188000000382 0.0000000000000000 F F F 1.5707500785374719 4.5343646213230482 2.5394500034680880 F F F 1.5692364825693324 2.7189723476989545 5.1603251857645258 T T T 0.0000000000000551 5.4412375999999805 0.0000000000000000 F F F 0.000000785375054 7.2549834213229909 2.5394500034680880 F F F -0.0001238833096484 5.4272400989988236 5.1803935228972788 T T T -0.0072360600433719 7.5025952070031483 7.5211672511623698 T T T -1.5707499999999670 8.1618564000000191 0.0000000000000000 F F F -1.5707499214625162 9.9756022213230295 2.5394500034680880 F F F -1.5864847811982092 8.1834252566855259 5.0029748321410761 T T T -1.5680206745798797 10.1569812891122950 7.685173732659610 T T T -3.1414999999999336 10.8824751999999609 0.0000000000000000 F F F -3.1414999214625388 12.6962210213230691 2.5394500034680880 F F F -3.1428198675740737 10.8880339067804197 5.0712888100552851 T T T -3.1443744630428521 12.8301353762893626 7.5779714843804622 T T T 6.2829999999999773 0.0000000000000000 0.0000000000000000 F F F 6.2830000785375404 1.8137458213230107 2.5394500034680880 F F F 6.2858619024005451 0.0264479510680984 5.086119007478505 T T T 4.7122499999999556 2.7206188000000382 0.0000000000000000 F F F 4.7122500785375179 4.5343646213230482 2.5394500034680880 F F F 4.7099375038894493 2.7092634600894825 5.1566119408179993 T T T 3.1414999999999886 5.4412375999999805 0.0000000000000000 F F F 3.1415000785375513 7.2549834213229909 2.5394500034680880 F F F 3.1432386200448736 5.4217420388173609 5.1270431578998341 T T T 1.5707499999999666 8.1618564000000191 0.0000000000000000 F F F 1.5707500785375297 9.9756022213230295 2.5394500034680880 F F F 1.609042376447873 8.1474110852702263 5.1086424458294939 T T T 1.5809556849571174 10.08526724253095440 7.6335787068075852 T T T 0.0000000000000000 10.8824751999999609 0.0000000000000000 F F F 0.0000007853750772 12.6962210213230691 2.5394500034680880 F F F 0.0068764382867794 10.8748590305724484 5.0686883826187250 T T T 0.8122906733910968 12.797658907696205 7.5807123309364055 T T T 9.4245000000000214 0.0000000000000000 0.0000000000000000 F F F 9.4245000785374717 1.8137458213230107 2.5394500034680880 F F F 9.4323256159073143 0.0303125677957576 5.099214572441038 T T T 7.8537499999999998 2.7206188000000382 0.0000000000000000 F F F

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Selective dynamics
Cartesian
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