Table 1. The sorption efficiency of PGMs/Mo ions into PBNPs, the elution efficiency of Fe ion from PBNPs after 24 h sorption test, the substitution efficiency of PGMs/Mo with Fe2+ or Fe3+ ion, the substitution site, and the amount of recovery per 1 g PB.

	Ru	Rh	Pd	Mo
Sorption efficiency [%]	33.1	68.2	99.9	51.7
Elution efficiency of Fe ion [%]	19.5	23.9	43.5	17.1
Substitution efficiency [%]	39.0	47.8	87.0	17.1
Substitution site	Fe^{3+}	Fe^{3+}	Fe^{2+}	Fe^{2+}/Fe^{3+}
Amount of recovery per 1g PB* [g]	0.128	0.160	0.302	0.107

*Chemical form: $KFe(III)[Fe(II)(CN)_6]$

$$\textbf{Sorption efficiency [\%]} = [(C_{initial} - C_{final})/C_{initial}] \times 100$$

Here, $C_{initial}$ and C_{final} denote the concentration of Pd ion in nitric acid solution before and after 24-h sorption test, respectively.

Table 2. The crystallite size and lattice constant of the pristine and PGMs/Mo-sorbed PBNPs.

	Crystallite size [nm]	Lattice constant [Å]
Pristine PB	16.1	10.16
Ru-sorbed PB	16.3	10.21
Rh-sorbed PB	16.7	10.21
Pd-sorbed PB	16.7	10.21
Mo-sorbed PB	16.7	10.21

Table 3. The adsorption energy, diffusion barrier, and substitution energy of PGMs/Mo ions when incorporated into PB unit cells.

	Adsorption energy [eV]	Diffusion barrier [eV]	Substitution energy [eV]
Ru^{4+}	1.8	4.0	– 1.2 (Fe^{2+}) / – 4.1 (Fe^{3+})
Rh^{3+}	0.2	3.8	– 0.9 (Fe^{2+}) / – 1.5 (Fe^{3+})
Pd^{2+}	0	2.5	– 0.9 (Fe^{2+}) / + 0.6 (Fe^{3+})
Mo^{6+}	3.2	8.0	+ 3.8 (Fe^{2+}) / – 2.8 (Fe^{3+})