Supplementary Information

Machine learning to predict the interfacial behavior of pesticide droplet on hydrophobic surfaces for minimizing environmental risk

Ridan Song[†], *Yanling Wu*[†], *Zhenping Bao*[†], *Yuxia Gao*[†], *Kefei Zhao*[†], *Songhao Zhang*[†], *Chenhui Zhang*[†,*], and *Fengpei Du*[†,*]

† Affiliation 1: Department of Applied Chemistry, College of Science, China Agricultural University, Yuanmingyuan West Road 2, Haidian District, Beijing, 100193, China

* Corresponding authors

Email addresses: dufp@cau.edu.cn (F. Du)

zhch@cau.edu.cn (C. Zhang)

The Supplementary Information contains 13 pages, 4 tables, 7 figures and 1 movie.

List of Figures, Tables and Movies:

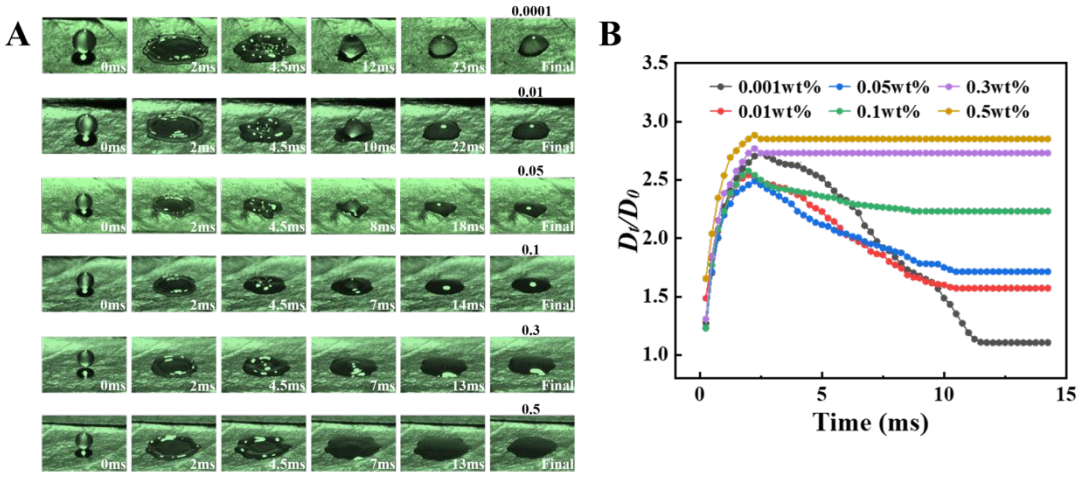

Figure S1. The impact process (A) and normalized contact radius (B) of AOT droplets with different concentrations of 0.0001, 0.01, 0.05, 0.1, 0.3, 0.5wt% on the *C. reticulata* Blanco Ⅰ leaf surfaces. The state of the six images from left to right is just approaching contact, maximum diffusion, receding, maximum bounce height, deposition and deposition state after 1 min.

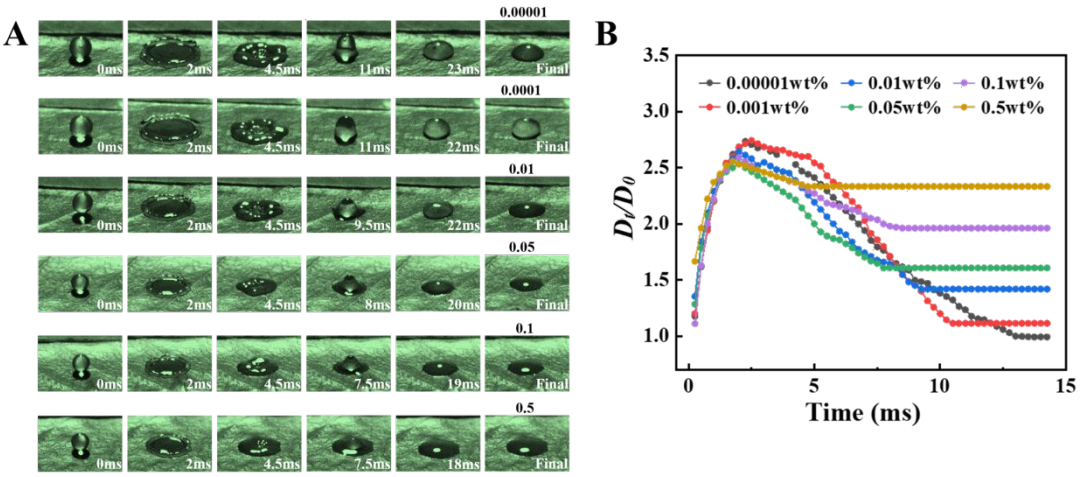

Figure S2. The impact process (A) and normalized contact radius (B) of AEO droplets with different concentrations of 0.00001, 0.0001, 0.01, 0.05, 0.1, 0.5wt% on the *C. reticulata* Blanco Ⅰ leaf surfaces. The state of the six images from left to right is just approaching contact, maximum diffusion, receding, maximum bounce height, deposition and deposition state after 1 min.

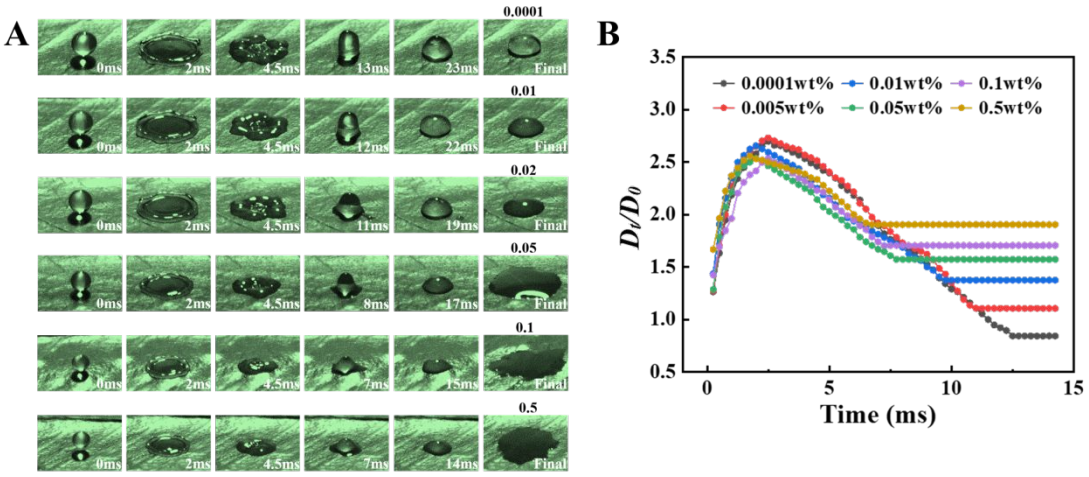

Figure S3. The impact process (A) and normalized contact radius (B) of L-77 droplets with different concentrations of 0.0001, 0.01, 0.02, 0.05, 0.1, 0.5wt% on the *C. reticulata* Blanco Ⅰ leaf surfaces. The state of the six images from left to right is just approaching contact, maximum diffusion, receding, maximum bounce height, deposition and deposition state after 1 min.

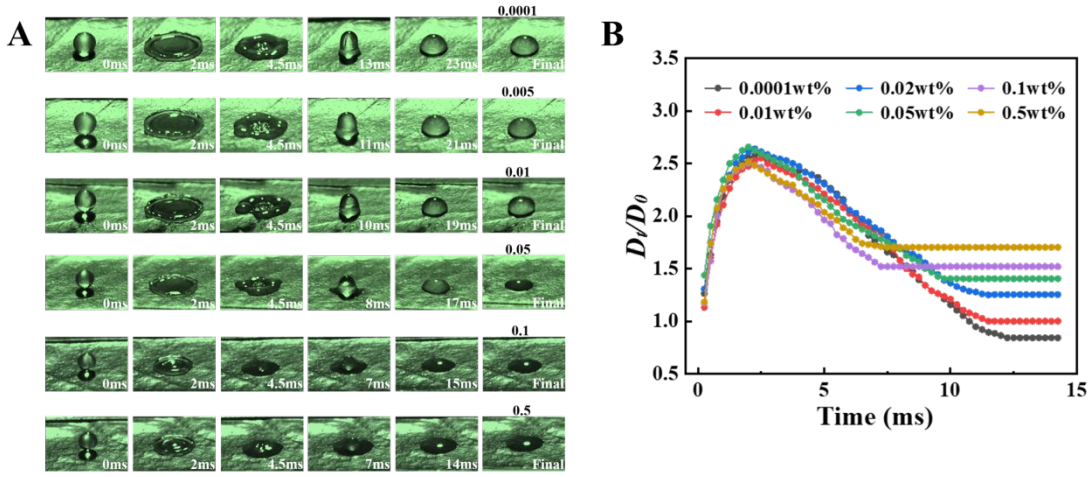

Figure S4. The impact process (A) and normalized contact radius (B) of CAPB droplets with different concentrations of 0.0001, 0.005, 0.01, 0.05, 0.1, 0.5wt% on the *C. reticulata* Blanco Ⅰ leaf surfaces. The state of the six images from left to right is just approaching contact, maximum diffusion, receding, maximum bounce height, deposition and deposition state after 1 min.

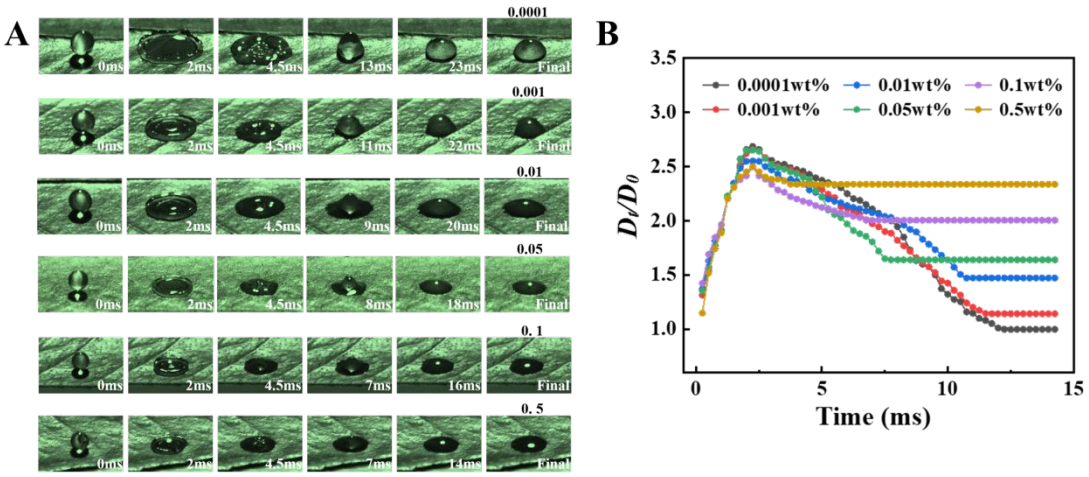

Figure S5. The impact process (A) and normalized contact radius (B) of APG droplets with different concentrations of 0.0001, 0.001, 0.01, 0.05, 0.1, 0.5wt% on the *C. reticulata* Blanco Ⅰ leaf surfaces. The state of the six images from left to right is just approaching contact, maximum diffusion, receding, maximum bounce height, deposition and deposition state after 1 min.

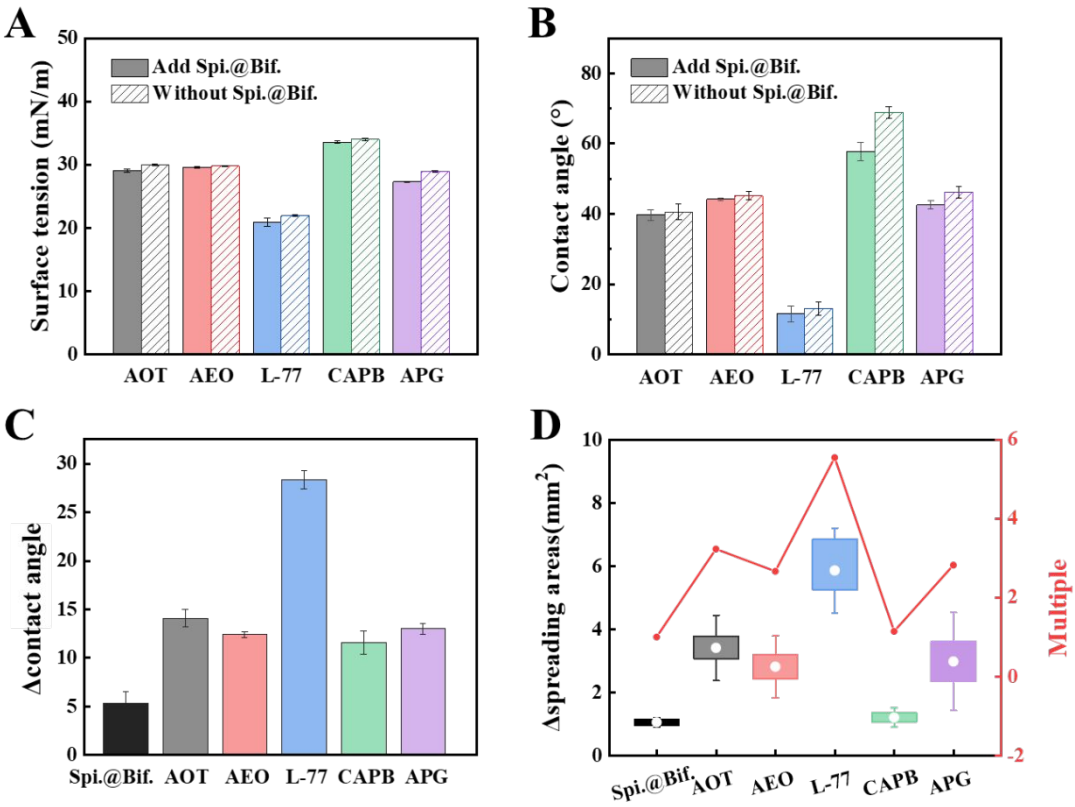

Figure S6. Performance after adding pesticide liquids. Changes of equilibrium surface tension (A) and contact angle (B) before and after adding Spi.@Bif. The change of contact angle (C) and wetting areas within 1 min (D) of pesticide liquids on the *C. reticulata* Blanco Ⅰ leaf surfaces.

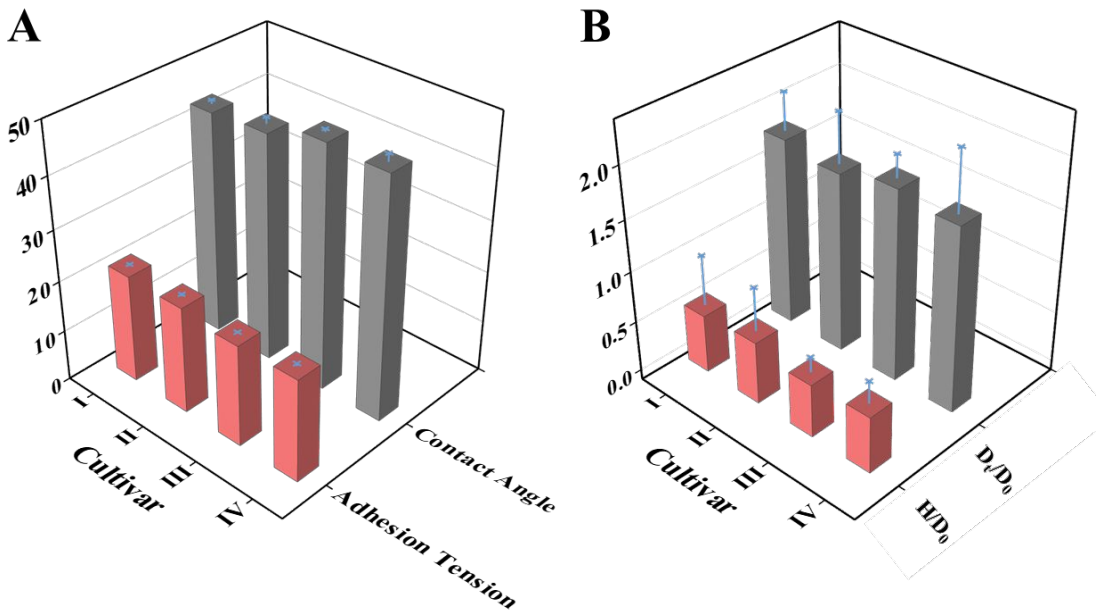

Figure S7. Effect of *C. reticulata* Blanco cultivars on contact angle and adhesion tension (A), normalized contact radius and normalized rebound height (B).

Table S1. Test liquids and their surface tension.

Test liquid	Total surface tension (mJ/m^2)	Dispersion component (mJ/m^2)	Polar component (mJ/m^2)
Water	72.80	29.10	43.70
Formamide	58.20	35.10	23.10
Ethylene glycol	48.20	29.29	18.91
Diiodomethane	50.80	50.42	0.38

Table S2. Effect of *C. reticulata* Blanco cultivars on surface free energy and its components. Note: df, degrees of freedom; SS, sum of squares; MS, mean square; F, test statistics; P, probability value.

Source	df	SS	MS	F	P
Surface free energy	1	1.058	1.058	1.108	0.403
Dispersion component	1	0.558	0.558	0.369	0.606
Polar component	1	0.049	0.049	0.585	0.524

Table S3. Surface activity and thermodynamic parameters of surfactants.

Surfactant	CMC (wt%)	π_{CMC} (mN/m)	Γ_m (μmol/m^2)	ΔG^{θ}_{mic} (kJ/mol)	ΔG^{θ}_{ad} (kJ/mol)
AOT	0.1	45.52	1.21	-25.07	-61.46
AEO	0.05	42.20	2.41	-26.56	-42.88
L-77	0.05	50.06	2.84	-27.57	-42.25
CAPB	0.005	37.05	3.42	-31.84	-41.14
APG	0.005	42.91	3.06	-31.89	-43.28

Table S4. The viscosity of five surfactant solutions.

	Water	0.05wt% AOT	0.05wt% AEO	0.05wt% L-77	0.05wt% CAPB	0.05wt% APG
Viscosity (mPa s)	1.02±0.03	1.05±0.03	1.04±0.05	1.06±0.06	1.04±0.03	1.11±0.04