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Supporting Information

Quantitative and High-resolution Mechanical Pressure Sensing Functions of Mechanochromic Fluorenylidene-Acridane

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<u>1. Experimental Section</u>

1.1. Materials and Synthesis. Materials were purchased from Tokyo Kasei Industry Co., Ltd., Sigma-Aldrich Inc., and other commercial suppliers and used after appropriate purification before use. Anhydrous solvents (stabilizer-free) were purchased from FUJIFILM Wako Pure Chemical Corporation. All reactions dealing with air- or moisture-sensitive compounds were carried out in a dry reaction vessel under nitrogen or argon. All reactions were monitored by thin layer chromatography (TLC, eluent, $CHCl_3$). Compound 1 was obtained by Barton-Kellogg reaction using diazofluorenylidene and thioacridane (Scheme S1). Diazofluorenylidene (1.90 g, 5.89 mmol) and triphenylphosphine (3.71 g, 14.1 mmol) was added in two-necked flask. Thioacridane dissolved in oxylene was dropped in the flask at 140 °C for 1 hour. Reaction temperature was decreased to room temperature and the solvent was removed by evaporator. The solid products were charged on a silica gel short column to remove some impurities using dichloromethane as eluent. Then, triethylamine/dichloromethane mixture (1/5) was passed to collect the crude. Second silica gel column which was prepared with trimethylamine was performed using n-hexane/dichloromethane (1/5) as eluent to obtain the pure twisted conformer of 1. The folded conformer of 1 (1.19g, 2.47 mmol) was generated from the twisted conformer in methanol by sonication (Figure S1). The product was verified by NMR spectra (JEOL ECA-600).



Scheme S1. Synthesis of mechanochromic fluorenylidene-acridane 1.



Figure S1. Photographs of sonication which converted the twisted conformer of **1** into the folded conformer.

1.2. Film preparation and nanoimprinting technique. The glass substrates were washed with a cleaning solution ($NH_3:H_2O_2:H_2O = 1:1:5$) at 75 °C for 5 min, rinsed with deionized water. And then, the substrates were dried using a N_2 gun and subjected to 20 min UV/O₃ treatment (BioForce Nanosciences ProCleaner 100). The silicon substrates were cleaned by Ar^+ ion sputtering apparatus, Elionix EIS-230 and subjected to 20 min UV/O₃ treatment (BioForce Nanosciences ProCleaner 100). Vacuum deposition films were prepared using a ULVAC VPC-410 vacuum evaporator. Thickness of those films was measured by a surface profiler, Bruker Dektak XT. Quantitative mechanical pressure was applied on a nanoimprinting instrument (SCIVAX X-300). The nanoimprinting treatment was performed for 360 sec at 25 °C after the pressure value reached to the set point.

1.3. Preparation for patterned silicon mold. Silicon substrates were cleaned with oxygen plasma using reactive ion etching apparatus (Samco Inc. RIE-10NRT). Positive photoresist was spin-coated on the silicon substrate with 3000rpm for 20sec. A wafer was bake at 90 °C for 90 sec for pre-exposure bake. The exposure was done with maskless exposure system, NanoSystem Solutions Inc. DL-1000. Then, post-exposure bake was performed on hot plate at 110 °C for 90sec. The silicon substrates were immersed in NMD-3 solution for 60 sec and rinsed in pure water. Al was deposited on patterned silicon substrate using a sputtering apparatus (;Elionix Inc. EIS-230). Thereafter, lift-off process was performed by immersion in acetone and ultrasonic cleaning.

1.4. Measurement information. UV-Vis absorption spectra were recorded on a JASCO V-670 spectrometer. We used a slit to narrow measurement spots to Φ 5 mm for the sample area of 1 cm². The data were averaged from 4 times measurements per each sample area. AFM and KFM images were taken on a scanning probe microscope, SHIMADZU SPM-9700.A silicon cantilever (OLYMPUS OMCL-AC240TS-C3) was employed for surface potentials measurements. KFM studies was performed with the standard noncontact AFM setup in air. In these measurements, samples and the cantilever were treated with electrostatic removal by the ionizer. Surface potentials were calculated as the average from 4 times measurements per each sample area. The surfaces of blue/yellow films were observed by digital microscope (Keyence VHX-2000). Ionization potential was measured by a photoelectron yield spectrometer, RIKEN KEIKI AC-3 PYS in air. Thermogravimetry differential thermal analysis (TG-DTA) was performed on a thermal analyzer, SHIMADZU DTG-60. XRD analyses was performed on an X-ray diffractometer, Rigaku SmartLab. Reflectance IR spectroscopy of films were measured using JASCO FT/IR-6100 and IRT-5200. Scratch tests of a PVA sheet containing **1** was investigated by friction tester, Trinity-Lab. I-tester TL201Tt.

2. Photographs of cast-deposition of 1



Figure S2. Photographs of cast-deposition. (a) 1: 50 mg/mL, THF : PGMEA = 1 : 1. (b) 1: 50 mg/mL, dichloromethane : PGMEA = 1 : 1. (c) 1: 50 mg/mL, CHCl₃ : PGMEA = 1 : 1. (d) 1: 12.5 mg/mL, PGMEA. (e) 1: 25 mg/mL, PGMEA. (f) 1: 50 mg/mL, PGMEA. PGMEA is propylene glycol monomethyl ether acetate.





Figure S3. TG-DTA data for **1**. Blue and red lines represent thermogravimetry and differential thermal analysis.

4. Photographs of vapor exposure of 1 to methanol



Figure S4. Photographs of vapor exposure of **1** to methanol on plastic films. (a) Low density polyethylene. (b) High density polyethylene. (c) Polypropylene.



5. UV-Vis spectra of films of 1

Figure S5. (a) Diffuse reflectance UV-Vis spectra for films of 1 under various mechanical pressure.(b) Plot of reflectance at 680 nm versus mechanical pressure.



6. Investigation for repeatability and reliability of mechanochromism

Figure S6. Repeatability cycle tests with repeated mechanical pressure application and MeOH vapor exposure. (a) Diffuse reflectance UV-Vis spectra of films of **1**. The average spectrum of 3 times per each sample were represented. (b) Plot of reflectance versus mechanical pressure and vapor exposure cycles. The reflection coefficients were normalized to the first yellow film. (c) KFM images of films. The measurements were done 3 times per each sample. (d) Plot of potential difference versus mechanical pressure and vapor exposure cycles. The surface potentials were offset to the first yellow film.

7. Explanation of observation for spatial resolution



Figure S7. (a) Cross section image of two silicon molds. (b) Photographs of a wide scale silicon mold. (c) AFM image of a narrow scale silicon mold. (d) Illustration for investigation of spatial resolution using the molds.

8. AFM images



Figure S8. AFM images (10 x 10 µm). (a) Blue film. (b) Yellow film.



Figure S9. Digital microscope images. (a) Blue film. (b) Yellow film.

10. Reflectance infrared absorption spectrometry

In the peak at 1600 cm⁻¹ derived from vibration of aryl rings of the fluorenyl unit, the yellow film gave broader peak. This difference indicates strong intermolecular interaction observed in the polycrystalline yellow film.



Figure S10. IR spectra for the blue film (blue line) and the yellow film (yellow line).

<u>11. XRD patterns</u>



Figure S11. XRD patterns for the blue film (blue line) and the yellow film (yellow line). Inset pictures are blue and yellow film samples for these measurements.



Figure S12. XRD patterns for blue powder (blue line), green powder (green line), and yellow powder (yellow line).

<u>12. Photoelectron yield spectra</u>



Figure S13. PYS spectra for a blue film (blue dots) and yellow a film (yellow dots).

13. DFT studies

Table S1. Cartesian coordinates for the optimized structure of compound 1 in each conformation.

1. Folded monomer

1.	1. Folded monomer		Н	-9.40233149000	0.52403428000	-1.07069204000	
Syı	mbol X	Y	Z	Н	-8.27950957000	1.79135289000	0.74174906000
С	-7.16837998000	-1.32790221000	1.52155788000	Н	-7.61177197000	-3.10655660000	0.37859570000
С	-7.28237321000	0.08342296000	1.57057401000	С	-5.49469658000	2.65123456000	1.20642361000
N	-6.51464118000	-1.98149967000	2.58796659000	С	-4.94119668000	2.61387085000	3.50904670000
С	-6.53296333000	0.77932407000	2.64352782000	С	-4.83776801000	3.86668107000	1.53583900000
С	-6.60000557000	-1.37159291000	3.85760923000	С	-4.49722801000	3.84395398000	2.95454026000
С	-6.71285153000	0.03976264000	3.91552723000	С	-5.69187260000	2.34059535000	-0.13827007000
С	-7.74460348000	-2.03365457000	0.45239025000	С	-4.50665530000	2.26018908000	4.78591655000
С	-6.16063932000	-3.36907134000	2.47378163000	С	-4.48775023000	4.78072194000	0.54937712000
С	-8.13476665000	0.71939962000	0.65702467000	С	-3.73469125000	4.73237892000	3.70341156000
С	-6.62483817000	-2.11836038000	5.04723777000	С	-3.34308907000	4.39434571000	5.00206858000
С	-5.73598945000	1.88050374000	2.46993253000	С	-3.69990580000	3.14437686000	5.52163283000
С	-7.04534003000	0.63627991000	5.13987364000	Н	-4.73670596000	1.30675462000	5.23977434000
С	-4.84801500000	-3.70501777000	2.13164425000	Н	-3.39482983000	5.67052020000	3.27374371000
С	-7.10505676000	-4.37910308000	2.69519175000	С	-4.73131040000	4.48597482000	-0.79513839000
С	-6.73306425000	-5.71881694000	2.57453654000	С	-5.30118694000	3.25255669000	-1.13343288000
С	-4.48020967000	-5.04618221000	2.01141556000	Н	-6.11410457000	1.40165865000	-0.46720814000
С	-5.42095731000	-6.05375102000	2.23247974000	Н	-3.98138617000	5.70691668000	0.80584433000
Н	-8.12298850000	-4.10746930000	2.95921845000	0	-3.29002859000	2.67488918000	6.74499357000
Н	-7.46854509000	-6.49983521000	2.74722737000	0	-5.50921635000	2.82813452000	-2.42167170000
Н	-4.12826620000	-2.90985267000	1.96278981000	Н	-2.72661277000	5.08248544000	5.56757515000
Η	-3.45854018000	-5.30233066000	1.74486612000	Н	-4.42995908000	5.19416312000	-1.55756882000
Η	-5.13339363000	-7.09740747000	2.13865828000	С	-2.41251262000	3.48749202000	7.50866496000
С	-7.13329231000	-0.11332210000	6.30825407000	Н	-1.48144796000	3.70221660000	6.96721422000
С	-6.88074368000	-1.48765755000	6.26057900000	Н	-2.88833407000	4.43529456000	7.79644867000
Η	-7.20491096000	1.70904254000	5.16774064000	Н	-2.18487729000	2.91488506000	8.41038162000
Η	-7.37819640000	0.37050225000	7.24914069000	С	-5.07922582000	3.67075754000	-3.47864211000
Η	-6.91456426000	-2.08173431000	7.17000458000	Н	-5.61165653000	4.63203638000	-3.47138202000
Η	-6.48052213000	-3.19186175000	5.01554479000	Н	-3.99775318000	3.85838761000	-3.43774872000
С	-8.75669300000	0.00980904000	-0.36495231000	Н	-5.31939591000	3.13770607000	-4.40119058000
С	-8.52370249000	-1.36352265000	-0.48541922000				
Н	-8.97760887000	-1.92623045000	-1.29685523000	2.	Twisted mono	mer	

S11

Syı	mbol X	Y	Z	
С	-0.458231000	0.181377000	-0.425719000	
С	-0.828029000	1.549066000	-0.274649000	
Ν	0.323208000	-0.452964000	0.545316000	
С	-0.407577000	2.309399000	0.904462000	
С	0.683917000	0.197638000	1.728335000	
С	0.308225000	1.553093000	1.932889000	
С	-0.836637000	-0.528767000	-1.585240000	
С	0.741165000	-1.815571000	0.337502000	
С	-1.458347000	2.164183000	-1.382455000	
С	1.376712000	-0.502735000	2.738122000	
С	-0.650008000	3.686321000	1.057960000	
С	0.507500000	2.086972000	3.228192000	
С	1.965644000	-2.078742000	-0.281816000	
С	-0.075915000	-2.868743000	0.757976000	
С	0.334492000	-4.187272000	0.556400000	
С	2.372671000	-3.399119000	-0.479490000	
С	1.558383000	-4.453807000	-0.061469000	
Н	-1.024569000	-2.645941000	1.237266000	
Н	-0.301543000	-5.005467000	0.882649000	
Н	2.587832000	-1.248724000	0-0.602872000	
Н	3.325101000	-3.602427000	0-0.960901000	
Н	1.876649000	-5.480900000	0-0.216899000	
С	1.161734000	1.388298000	4.226072000	
С	1.626438000	0.092680000	3.964418000	
Н	0.120444000	3.072789000	3.446315000	
Н	1.278548000	1.841948000	5.204968000	
Н	2.152615000	-0.470001000	4.731051000	
Н	1.698410000	-1.521106000	2.560609000	
С	-1.818681000	1.464929000	-2.519492000	
С	-1.523231000	0.098948000	-2.610461000	
Н	-1.804062000	0-0.470396000	-3.492335000	
Н	-2.309518000	1.980622000	-3.339498000	
Н	-1.657468000	3.225491000	-1.334465000	
Н	-0.577335000	0-1.575507000	-1.678332000	
С	0.322697000	4.698092000	1.514896000	

С	-1.896252000 4.426615000 0.798570000
С	-0.295141000 5.982356000 1.478843000
С	-1.687025000 5.805634000 1.090616000
С	1.692262000 4.608058000 1.779660000
С	-3.193532000 3.975797000 0.531184000
С	0.445243000 7.127586000 1.753454000
С	-2.749164000 6.702939000 1.046525000
С	-4.036161000 6.254278000 0.740446000
С	-4.254106000 4.887615000 0.502045000
Η	-3.415445000 2.928985000 0.354083000
Η	-2.592445000 7.754702000 1.274011000
С	1.807769000 7.029828000 2.053352000
С	2.426163000 5.768003000 2.053619000
Η	2.218579000 3.660156000 1.791136000
Η	-0.024394000 8.107954000 1.722373000
0	3.760877000 5.566212000 2.312448000
0	-5.489081000 4.342889000 0.236998000
Η	2.374839000 7.929646000 2.262548000
Η	-4.857650000 6.960285000 0.723604000
С	4.575157000 6.698800000 2.545424000
Η	4.576636000 7.384594000 1.686816000
Η	4.259993000 7.253307000 3.440861000
Η	5.586525000 6.316419000 2.700697000
С	-6.620041000 5.199426000 0.280290000
Η	-6.734222000 5.668511000 1.265412000
Η	-6.564104000 5.979618000 -0.491440000
Н	-7.485087000 4.562827000 0.083144000

3. Folded dimer

Sy	mbol X	Y	Z
С	-0.98717900000	0.13988100000	0.25863900000
С	-1.54339200000	1.42939900000	0.39038700000
N	-0.11147400000	-0.31469600000	1.26238300000
С	-1.00595100000	2.27297800000	1.47296500000
С	-0.33170000000	0.17605800000	2.56202200000
С	-0.88624300000	1.46445100000	2.69929300000

С	-1.34972600000	-0.66011200000	-0.83076100000	С	1.09006800000	6.50432900000	3.96118900000
С	0.56788000000	-1.55978300000	1.08131500000	С	1.11022100000	5.18391100000	4.41080200000
С	-2.59367100000	1.79660700000	-0.45306100000	Н	0.64647700000	3.14572000000	4.04313100000
С	-0.05621200000	-0.58198600000	3.70555100000	Н	0.60425000000	7.80535700000	2.31907800000
С	-0.59535700000	3.56785400000	1.34531500000	С	-0.67341900000	6.54537000000	-1.72647800000
С	-1.34123800000	1.87008700000	3.95523900000	С	-0.91708500000	5.23159300000	-2.12709700000
С	1.88871300000	-1.55161300000	0.64669200000	Н	-1.09860300000	3.18624200000	-1.58965600000
С	-0.08612800000	-2.76905800000	1.31803800000	Н	-0.14206700000	7.82157000000	-0.07994900000
С	0.58758700000	-3.96837200000	1.12228300000	0	1.63628300000	4.79267900000	5.60400300000
С	2.55975500000	-2.75467400000	0.44958600000	0	-1.16280200000	4.85965500000	-3.41351700000
С	1.91070800000	-3.96146800000	0.68771800000	Н	1.49210900000	7.31031700000	4.56960400000
Н	-1.12397100000	-2.75200300000	1.65060900000	Н	-0.68328500000	7.36229300000	-2.44334200000
Η	0.07808000000	-4.91252400000	1.30644800000	С	2.21478600000	5.77829800000	6.41696600000
Η	2.37501900000	-0.59463300000	0.46611800000	Н	3.04985200000	6.28704000000	5.91050600000
Н	3.59352600000	-2.74783800000	0.10936500000	Н	1.47787000000	6.53446300000	6.72996900000
Η	2.43591900000	-4.90233300000	0.53317400000	Н	2.59533500000	5.26462100000	7.30403400000
С	-1.13088000000	1.08911200000	5.08066900000	С	-1.12732300000	5.85622300000	-4.39993100000
С	-0.44739200000	-0.11878100000	4.95294600000	Н	-1.90280200000	6.62124300000	-4.23761900000
Н	-1.83532800000	2.83655600000	4.04079700000	Н	-0.14518900000	6.35230700000	-4.44306500000
Н	-1.47854100000	1.42817000000	6.05405800000	Н	-1.31648600000	5.35578200000	-5.35357400000
Н	-0.24041600000	-0.72594200000	5.83256700000	С	-6.02081483100	-1.45541497100	1.13984145800
Н	0.43465000000	-1.54764000000	3.61125400000	С	-6.57702783100	-0.16589697100	1.27158945800
С	-2.99713000000	0.97688000000	-1.49548500000	N	-5.14510983100	-1.90999197100	2.14358545800
С	-2.33967600000	-0.23375700000	-1.70317700000	С	-6.03958683100	0.67768202900	2.35416745800
Н	-2.62234800000	-0.87281200000	-2.53803500000	С	-5.36533583100	-1.41923797100	3.44322445800
Η	-3.80739800000	1.28615200000	-2.15212600000	С	-5.91987883100	-0.13084497100	3.58049545800
Н	-3.07223300000	2.76179200000	-0.29518500000	С	-6.38336183100	-2.25540797100	0.05044145800
Н	-0.87956600000	-1.62989400000	-0.97429700000	С	-4.46575583100	-3.15507897100	1.96251745800
С	-0.67993400000	4.44398300000	0.14247800000	С	-7.62730683100	0.20131102900	0.42814145800
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С	-0.36398200000	5.76830900000	0.52880300000	С	-5.62899283100	1.97255802900	2.22651745800
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С	0.57578400000	4.14904100000	3.63520500000	С	-5.11976383100	-4.36435397100	2.19924045800
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С	-3.12292783100	-5.55676397100	1.56892045800
Н	-6.15760683100	-4.34729897100	2.53181145800
Н	-4.95555583100	-6.50781997100	2.18765045800
Н	-2.65861683100	-2.18992897100	1.34732045800
Н	-1.44010983100	-4.34313397100	0.99056745800
Н	-2.59771683100	-6.49762897100	1.41437645800
С	-6.16451583100	-0.50618397100	5.96187145800
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Н	-6.86896383100	1.24126002900	4.92199945800
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Н	-4.59898583100	-3.14293597100	4.49245645800
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С	-7.37331183100	-1.82905297100	-0.82197454200
Н	-7.65598383100	-2.46810797100	-1.65683254200
Н	-8.84103383100	-0.30914397100	-1.27092354200
Н	-8.10586883100	1.16649602900	0.58601745800
Н	-5.91320183100	-3.22518997100	-0.09309454200
С	-5.71356983100	2.84868702900	1.02368045800
С	-5.02165883100	2.83581302900	3.27941745800
С	-5.39761783100	4.17301302900	1.41000545800
С	-4.96965083100	4.16488302900	2.79825745800
С	-5.95453883100	2.58815902900	-0.31861854200
С	-4.45785183100	2.55374502900	4.51640745800
С	-5.41382483100	5.20866802900	0.49180145800
С	-4.45703383100	5.18785302900	3.57755945800
С	-3.94356783100	4.90903302900	4.84239145800
С	-3.92341483100	3.58861502900	5.29200445800
Н	-4.38715883100	1.55042402900	4.92433345800
Н	-4.42938583100	6.21006102900	3.20028045800
С	-5.70705483100	4.95007402900	-0.84527554200
С	-5.95072083100	3.63629702900	-1.24589454200
Н	-6.13223883100	1.59094602900	-0.70845354200
Н	-5.17570283100	6.22627402900	0.80125345800
0	-3.39735283100	3.19738302900	6.48520545800
0	-6.19643783100	3.26435902900	-2.53231454200

Н	-3.54152683100	5.71502102900	5.45080645800
Η	-5.71692083100	5.76699702900	-1.56213954200
С	-2.81884983100	4.18300202900	7.29816845800
Η	-1.98378383100	4.69174402900	6.79170845800
Η	-3.55576583100	4.93916702900	7.61117145800
Н	-2.43830083100	3.66932502900	8.18523645800
С	-6.16095883100	4.26092702900	-3.51872854200
Н	-6.93643783100	5.02594702900	-3.35641654200
Н	-5.17882483100	4.75701102900	-3.56186254200
Н	-6.35012183100	3.76048602900	-4.47237154200

4. Twisted dimer

Syı	mbol X	Y	Z
С	-2.40803068800	-0.05288320500	1.69173735600
С	-2.58776868800	1.36463179500	1.58742035600
N	-1.43761168800	-0.58806120500	2.54893535600
С	-1.72288768800	2.25662279500	2.36210035600
С	-0.78158068800	0.20894879500	3.48894135600
С	-0.94378068800	1.62236079500	3.42801935600
С	-3.16937568800	-0.92924520500	0.88576535600
С	-1.10907068800	-1.98540620500	2.44327935600
С	-3.49283968800	1.81379379500	0.59210535600
С	0.01808331200	-0.37636020500	4.49535035600
С	-1.57032668800	3.63798279500	2.11563735600
С	-0.41110468800	2.38606879500	4.49745035600
С	-0.20822768800	-2.40231120500	1.45415235600
С	-1.70225868800	-2.91639820500	3.30471835600
С	-1.40244768800	-4.27747020500	3.16677735600
С	0.08899231200	-3.76421520500	1.31996935600
С	-0.50982768800	-4.70294220500	2.17303135600
Η	-2.38603868800	-2.56026420500	4.07026635600
Η	-1.87091068800	-5.00242720500	3.83359135600
Η	0.23928431200	-1.65790420500	0.79615935600
Η	0.78719831200	-4.09190420500	0.54900235600
Н	-0.27848468800	-5.76325420500	2.06432335600
С	0.34796031200	1.80464179500	5.50553235600

С	0.58643831200	0.41893479500	5.48642935600	Н	-6.56813768800	7.35523079500	2.91346835600
Η	-0.60433868800	3.45490579500	4.51733035600	Н	-6.95611568800	7.34603979500	1.15364535600
Η	0.74378431200	2.42389079500	6.31070235600	Н	-7.92650668800	6.36164179500	2.30825835600
Н	1.19248931200	-0.04866220500	6.26382935600	С	-5.35333200000	0.08748200000	2.67905600000
Η	0.17354831200	-1.45219420500	4.50197435600	С	-5.28121400000	1.49812700000	2.85549300000
С	-4.27115868800	0.94601979500	-0.16242564400	N	-4.65239600000	-0.74135400000	3.55594600000
С	-4.12039768800	-0.44028320500	-0.00317964400	С	-4.53796700000	2.09098500000	3.97051000000
Η	-4.72267068800	-1.13754520500	-0.58580564400	С	-3.71610400000	-0.22112600000	4.45804200000
Η	-4.98484768800	1.34747979500	-0.88038664400	С	-3.61595700000	1.19290500000	4.67029800000
Η	-3.57381368800	2.87801479500	0.40771635600	С	-6.10542900000	-0.46533900000	1.61895700000
Η	-2.99158468800	-1.99915520500	0.95346235600	С	-4.88499500000	-2.16170000000	3.52534600000
С	-0.27962968800	4.36075279500	2.11342035600	С	-5.86419300000	2.31057900000	1.85001900000
С	-2.59347968800	4.64939679500	1.81488735600	С	-2.91742600000	-1.11404000000	5.20810000000
С	-0.51792668800	5.73169379500	1.76713335600	С	-4.77710800000	3.43563900000	4.32671900000
С	-1.95792068800	5.92462279500	1.65017035600	С	-2.73242900000	1.61484100000	5.69646300000
С	1.03728331200	3.90449079500	2.24182535600	С	-4.11836000000	-2.97861400000	2.68609300000
С	-3.98893668800	4.59053679500	1.91509535600	С	-5.86963500000	-2.71339200000	4.35494400000
С	0.55140131200	6.61277679500	1.59989235600	С	-6.08132300000	-4.09809900000	4.34650100000
С	-2.72700268800	7.08469579500	1.53840035600	С	-4.32805800000	-4.36283400000	2.68558400000
С	-4.12790568800	7.01200479500	1.59891235600	С	-5.30906600000	-4.92338000000	3.51580900000
С	-4.75001768800	5.76413779500	1.79992535600	Η	-6.45202600000	-2.05486200000	4.99875600000
Η	-4.50834968800	3.66518379500	2.14109635600	Н	-6.84595700000	-4.53242400000	4.99144200000
Η	-2.24492968800	8.05821879500	1.42819835600	Н	-3.36914800000	-2.51591000000	2.05068500000
С	1.87025231200	6.16110979500	1.76862635600	Н	-3.72265500000	-4.99908300000	2.03881900000
С	2.10491131200	4.80543179500	2.08097635600	Η	-5.47350000000	-6.00164700000	3.51545200000
Η	1.27012831200	2.87118179500	2.48835335600	С	-1.91338400000	0.73549200000	6.39252600000
Η	0.37109631200	7.65590879500	1.33225935600	С	-1.99770000000	-0.64226100000	6.13853500000
0	3.35767431200	4.25650679500	2.25466035600	Н	-2.70458200000	2.66559300000	5.95758800000
0	-6.10898868800	5.58419979500	1.90816335600	Н	-1.22185900000	1.12035100000	7.14070500000
Η	2.69530731200	6.85868579500	1.64088135600	Н	-1.36770000000	-1.34843800000	6.68001600000
Η	-4.71780968800	7.92245379500	1.51765335600	Н	-3.03914500000	-2.18389000000	5.06078400000
С	4.47900331200	5.11642879500	2.10398535600	С	-6.58352200000	1.76526700000	0.79368500000
Η	4.53225931200	5.54420479500	1.08811435600	С	-6.72604300000	0.36967400000	0.69427900000
Η	4.46246531200	5.94045679500	2.83815735600	Н	-7.29595800000	-0.07080500000	-0.12517900000
Η	5.36159131200	4.49069179500	2.28114035600	Н	-7.02117500000	2.42155500000	0.04123300000
С	-6.92583068800	6.73894879500	2.07481735600	Н	-5.74481300000	3.38802200000	1.92214700000

Η	-6.18192500000	-1.54542200000	1.52032700000
С	-3.82158300000	4.48633800000	4.70712000000
С	-6.11256300000	4.07197000000	4.37677300000
С	-4.53918100000	5.70290500000	4.95881900000
С	-5.96296200000	5.42694500000	4.82098600000
С	-2.42518800000	4.52751500000	4.61098500000
С	-7.39817600000	3.54300000000	4.21271300000
С	-3.84872200000	6.90044900000	5.15490500000
С	-7.08589100000	6.22424400000	5.04597600000
С	-8.37315800000	5.70347800000	4.83917200000
С	-8.52099800000	4.36107600000	4.43115000000
Н	-7.56610300000	2.51661800000	3.89434300000
Н	-6.97227900000	7.25480400000	5.38825400000
С	-2.44633400000	6.92485900000	5.09650800000
С	-1.74355000000	5.73786100000	4.81251600000
Н	-1.84601800000	3.65776600000	4.32003600000
Н	-4.39415100000	7.83003700000	5.32978200000
0	-0.37541400000	5.65666100000	4.70076000000
0	-9.73659500000	3.74768400000	4.21413600000
Н	-1.91738700000	7.86411600000	5.24270100000
Н	-9.24082200000	6.33663000000	5.01217500000
С	0.36236100000	6.87188900000	4.61164700000
Н	-0.03553400000	7.51377200000	3.81139900000
Н	0.35077200000	7.41957100000	5.56967700000
Н	1.38641100000	6.57799500000	4.36023600000
С	-10.90965100000	4.52420400000	4.41573800000
Н	-10.99176600000	4.87762700000	5.45796300000
Н	-10.94278300000	5.39586600000	3.73942500000
Н	-11.7511680000	0 3.85852000000	4.19082300000



Figure S14. Optimized structures of **1**. (a) Folded monomer. (b) Twisted monomer. (c) Folded dimer. (d) Twisted dimer.

14. Yellowing of the blue film by vapor exposure to alcohols



Figure S15. Yellowing of a blue film by vapor exposure using alcohols (methanol, ethanol, isopropyl alcohol, and hexane from left).

Figure S16. Photographs representing the color change from yellow to green corresponding to mechanical pressure and the reverse color change from green to yellow by spraying ethanol.



16. Illustration and photographs of laminated yellow films

15. Photographs of reverse color change using ethanol

Figure S17. (a) Illustration of the cross section of a laminated yellow film fabricated on a plastic sheet. (b) Photographs of color change to green by mechanical pressure and reverse color change to yellow by contact with ethanol.

17. Scratch test of PVA sheets containing 1



Figure S18. A photograph of the scratch test.

Scratch area	Normal force [N]	Dynamic friction coefficient	Friction [N]
(a)	0.490	0.121	0.059
(b)	0.981	0.098	0.096
(c)	1.962	0.121	0.237
(d)	4.903	0.112	0.549
(e)	9.807	0.125	1.226

Table S2. Scratch test data of PVA sheet containing 1.

Preparation of the polyvinyl alcohol (PVA) sheets containing 1.

Compound 1 (50 mg) in a small amount of methanol was grinded in a mortar with a pestle. A suspension of 1 in methanol was added to a PVA (degree of saponification of 78–82 mol%) saturated aqueous solution (10 mL). After stirring for 12 h, aqueous dispersion was poured into a mold and warmed at 40 $^{\circ}$ C for 3 h.