**Table S5.** The proposed Chemicals for Additional AOP-based Hazard Evaluations in semiconductor manufacturing.

No	Chemicals	CAS No.	In Process	MIEs	KEs	AOs	GHS category	OSH Act	Chemicals control Ac	ACT ON THE SAFETY CONTROL tOF HAZARDOUS SUBSTANCES	WASTES CONTRO L ACT
1	1-Methoxy-2- propanol	107-98-2	Wafer processing, Photo (PR solvent)	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	1193 N/A, Breast Cancer	Flammable liquid Cat. 3	For Process safety management (PSM) Chemicals for exposure limits	N/A	Class 4 the second petroleum (Water- soluble (2,000 L)	Designated waste
2	1-nitronaphthalene	86-57-7	Intermediate for manufacturing branched light emitting agents for OLED devices	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	1193 N/A, Breast Cancer	Flammable solid Cat. 2 Acute toxic (Oral) Cat. 3 Chronic aquatic toxicity Cat. 2	N/A	Toxic	N/A	N/A
3	2,2',6,6'- Tetrabromobisphene 1 A	o 79-94-7	Semiconductor and other electronic component manufacturing	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	1193 N/A, Breast Cancer	Reproductive toxicity Cat. 1B Acute aquatic toxicity Cat. 1 Chronic aquatic toxicity Cat. 1	N/A	Toxic	N/A	N/A
4	2-Butoxyethanol	111-76-2	Overall Chip assembly	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	1193 N/A, Breast Cancer	Acute toxic (Oral) Cat. 4 Acute toxic (Inhalation: Vapor) Cat. 3 Skin corrosion/irritation Cat. 2 Serious eye damage/eye irritation Cat. 2 Carcinogenicity Cat. 2	Chemicals for working environment measurement (Eacl 6 months) Chemicals for management Chemicals for special health exam. (Each 12 months) Chemicals for exposure limits Chemicals for exposure limits Chemicals for	h N/A	Class 4 the second petroleum (Water- soluble) (2,000 L)	Designated waste
5	2-Methoxyethanol	109-86-4	Manufacture wafers for semiconductor manufacturing	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	1193 N/A, Breast Cancer	Cat. 4 Reproductive toxicity Cat. 1B Specific target organ toxicity	management For Process safety management (PSM) Chemicals for	Toxic	Class 4 the second petroleum (Water- soluble) (2,000 L)	Designated waste
6	4-Chloro-2- methylphenol	1570-64-5	Semiconductor Manufacturing	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	1193 N/A, Breast Cancer	Acute toxic (inhalation: dust/mist) Cat. 3 Skin corrosion/irritation Cat. 1 Germ cell mutagenicity Cat. 1B Acute aquatic toxicity Cat. 1 Chronic aquatic toxicity Cat. 1	exposure limits  N/A	N/A	N/A	Designated waste
7	9-Bromoanthracene	1564-64-3	Intermediate for manufacturing OLEI emitters	Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	1193 N/A, Breast Cancer	No data	N/A	N/A	N/A	N/A
8	Acetaldehyde	75-07-0	Mold, Chip assembly	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	1193 N/A, Breast Cancer	Flammable liquid Cat. 1 Acute toxic (Oral) Cat. 4 Serious eye damage/eye irritation Cat. 2 Germ cell mutagenicity Cat. 2 Carcinogenicity Cat. 1B Specific target organ toxicity (Single exposure) Cat. 3 (Respiratory irritation)	special health exam. (Each 12 months) For Process safety management (PSM) Chemicals for	N/A	Class 4 Special flammable (50 L)	Designated waste
9	Acetonitrile	75-05-8	Semiconductor Electrodes	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	1193 N/A, Breast Cancer	Flammable liquid Cat. 2 Acute toxic (Oral) Cat. 4 Serious eye damage/eye irritation Cat. 2 Specific target organ toxicity (Single exposure) Cat. 3 (Respiratory irritation)		N/A	Class 4 the first petroleum (Water- soluble) (400 L)	N/A

10	Antimony trichlorid	e10025-91-9	Semiconductor Manufacturing	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	1193 N/A, Breast Cancer	Corrosive to metal Cat. 1 Acute toxic (Oral) Cat. 4 Serious eye damage/eye irritation Cat. 2 Chronic aquatic toxicity Cat. 2	exam. (Each 12 months) For Process safety management (PSM) Chemicals for exposure limits Chemicals for working environment measurement Chemicals for working environment measurement. (Each 6 months) Chemicals for special health exam. (Each 12 months) Chemicals for special health exam. (Each 12 months) Chemicals for special health exam. (Each 12 months) Chemicals for exposure limits Chemicals for special health exam. (Each 12 months)	Toxic	N/A	Designated waste
11	Arsenic trioxide	1327-53-3	Semiconductor Manufacturing	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	1193 N/A, Breast Cancer	Acute toxic (Oral) Cat. 2 Serious eye damage/eye irritation Cat. 1 Carcinogenicity Cat. 1A Specific target organ toxicity (Single exposure) Cat. 3 (Respiratory irritation) Acute aquatic toxicity Cat. 1 Chronic aquatic toxicity Cat. 1	working environment measurement Chemicals for working environment measurement. (Each 6 months) Chemicals for special health	Toxic	N/A	Designated waste
12	Bisphenol A	80-05-7	Packaging	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	1193 N/A, Breast Cancer	Serious eye damage/eye irritation Cat. 1 Skin sensitization Cat. 1 Reproductive toxicity Cat. 1B	Chemicals for exposure limits	Toxic	N/A	N/A
13	Catechol	120-80-9	Wafer processing, Photo (PR removal)	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	Cancer	Acute toxic (Oral) Cat. 3 Acute toxic (dermal) Cat. 3 Skin corrosion/irritation Cat. 2 Serious eye damage/eye irritation Cat. 1 Germ cell mutagenicity Cat.	Chemicals for exposure limits	N/A	N/A	Designated waste
14	Cumene	98-82-8	Substitute for benzene in direct photocatalytic hydroxylation (of benzene)	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	1193 N/A, Breast Cancer	Specific target organ toxicity (Single exposure) Cat. 3 (Respiratory irritation)	For Process safety management (PSM) Chemicals for exposure limits	N/A	Class 4 the second petroleum (Insoluble) (1,000 L)	Designated waste
15	Diethanolamine	111-42-2	Used to remove unnecessary photoresist layers after turning and developing	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	1193 N/A, Breast Cancer	Acute toxic (Oral) Cat. 4 Skin corrosion /irritation Cat. 2 Serious eye damage/eye irritation Cat. 2 Carcinogenicity Cat. 2 Specific target organ toxicity	Chemicals for working environment measurement. (Each 6 months) Chemicals for management Chemicals for	N/A	Class 4 the third petroleum (Water- soluble) (4,000 L)	Designated waste
16	Diethylene glycol monobutyl ether	112-34-5	Semiconductor Manufacturing	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	1193 N/A Breast	Serious eye damage/eye	Chemicals for exposure limits	N/A	Class 4 the third petroleum (Water- soluble) (4,000 L)	N/A
17	Dimethyl acetamide	127-19-5	Photo(diluent)	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	1193 N/A, Breast Cancer	Acute toxic (inhalation: Vapor) Cat. 3 Serious eye damage/eye irritation Cat. 2	Chemicals for working environment measurement. (Each 6 months) Chemicals for	Toxic	Class 4 the second petroleum (Water- soluble) (2,000 L)	N/A

			Chip assembly, Chip		1182 Increase, Cell	Flammable liquid Cat. 2 Serious eye damage/eye irritation Cat. 2	management Chemicals for special health exam. (Each 6 months) Chemicals for special management Chemicals for exposure limits Chemicals for working environment measurement. (Each 6 months)	Toxic	Class 4 the first	
18	Ethyl acetate	141-78-6	adhesion, mold, Solder ball attachment, etc.	Activation, Estrogen receptor	1193 N/A, 1 Proliferation (Epithelial Cancer Cells)	(Single exposure) Cat. 3	Chemicals for management For Process safety management (PSM) Chemicals for exposure limits Chemicals for working environment	Chemicals for accident prep.	Class 4 the lins petroleum (Insoluble) (200 L)	Designated waste
19	Ethylene glycol	107-21-1	CVD, Dry etching, Wafer processing, Ion implantation	Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	Serious eye damage/eye irritation Cat. 2 Specific target organ toxicity (Single exposure) Cat. 3 (Respiratory irritation) Specific target organ toxicity (Single exposure) Cat. 2 Specific target organ toxicity	measurement. (Each 6 months) Chemicals for management Chemicals for special health exam. (Each 12	N/A	Class 4 the third petroleum (Water- soluble (4,000 L)	Designated waste
20	Glycerol	56-81-5	Chip assembly, Solder ball attachment	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	Breast No data	Chemicals for exposure limits	N/A	Class 4 the third petroleum (Water- soluble (4000 £)	N/A
21	Hexamethyldisilazar e	<sup>1</sup> 999-97-3	HMDS was used to silanize the surface of silcon wafer	1181	1182 Increase, Cell Proliferation (Epithelial Cancer Cells)	Flammable liquid Cat. 2 Acute toxic (Oral) Cat. 4 Acute toxic (idermal) Cat. 3 Acute toxic (inhalation: Vapor) Cat. 3 Skin corrosion/irritation Cat. Breast 1 Serious eye damage/eye irritation Cat. 1 Specific target organ toxicity (Single exposure) Cat. 3 (Respiratory irritation) Chronic aquatic toxicity: Cat	(PSM)	N/A	Class 4 the first petroleum (Insoluble liquid) (200 L)	N/A
22	Hydroquinone	123-31-9	A Semiconductor and Fluorescence Dual- Mode Room- Temperature Ammonia Sensor Achieved by Decorating Hydroquinone into a Metal-Organic Framework	1 1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cancer Cells)	4 Acute toxic (Oral): Cat. 4 Serious eye damage/eye irritation: Cat. 1 Skin sensitization: Cat. 1 Germ cell mutagenicity: Cat. 2 2 Carcinogenicity Cat. 2 Specific target organ toxicity (Single exposure) Cat. 3	Chemicals for working environment measurement. (Each 6 months) Chemicals for management Chemicals for special health exam. (Each 12 months) Chemicals for	Toxic	N/A	Designated waste
23	Indium arsenide	1303-11-3	A semiconductor composed of indium and arsenic	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cancer Cells)	Breast -	-	-	-	-
24	Indium phosphide	2398-80-7	Manufacture of semiconductor wafer	1181 Activation,	1182 Increase, Cell Proliferation (Epithelial Cancer Cells)	Carcinogenicity Cat. 1B Reproductive toxicity Cat. 2 Breast Specific target organ toxicity (Single exposure) Cat. 2 Specific target organ toxicity	(Indium and its compounds (From	N/A	N/A	N/A

25	Methyl-3-methoxy propionate	3852-09-3	Wafer processing, Photo (PR solvent)	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cancer Cells)	<sup>st</sup> No data	N/A	N/A	N/A	Designated waste
26	Naphthalene	91-20-3	Simple organic semiconductor	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cancer Cells)	Flammable solid Cat. 2 Acute toxic (Oral) Cat. 4 at Carcinogenicity Cat. 2 Acute aquatic toxicity Cat. 1 Chronic aquatic toxicity Cat.	Chemicals for exposure limits	N/A	N/A	N/A
27	n-Butyl alcohol	71-36-3	Semiconductor Manufacturing	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cancer Cells)	Flammable liquid Cat. 3 Skin corrosion/irritation Cat. 2 Serious eye damage/eyest irritation Cat. 2 Specific target organ toxicity (Single exposure) Cat. 3 (Narcotic effect) Aspiration hazard Cat. 2	Chemicals for working environment measurement. (Each 6 months) Chemicals for management Chemicals for special health exam. (Each 12 months) For Process safety management (PSM) Chemicals for exposure limits	N/A	Class 4 the second petroleum (Insoluble) (1,000 L)	Designated waste
28	Nitrilotriacetic acid	139-13-9	Chemical Bath Deposition Of Group Ii-vi Semiconductor Thin Films For Solar Cels Applications	Activation, Estrogen	1182 Increase, Cell 1193 N/A, Brea Proliferation (Epithelial Cancer Cells)	Acute toxic (Oral) Cat. 4 Serious eye damage/eye irritation Cat. 2 Carcinogenicity Cat. 1B Specific target organ toxicity st; (Single exposure) Cat. 3 (Respiratory irritation) Specific target organ toxicity (Repeated exposure) Cat. 2 Chronic aquatic toxicity Cat. 3	N/A	N/A	N/A	N/A
29	Nitrobenzene	98-95-3	Semiconductor Manufacturing	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cancer Cells)	Acute toxic (Oral) Cat. 4 Acute toxic (dermal) Cat. 3 Acute toxic (inhalation: Vapor) Cat. 3 at Carcinogenicity Cat. 2 Reproductive toxicity Cat. 2 Specific target organ toxicity (Repeated exposure) Cat. 1 Chronic aquatic toxicity Cat. 3	Chemicals for working environment measurement. (Each 6 months) Chemicals for management Chemicals for special health exam. (Each 12 months) Chemicals for exposure limits	Toxic Chemicals for accident prep.	Class 4 the third petroleum (Insoluble) (2,000 L)	Designated waste
30	Pentaerythritol triacrylate	3524-68-3	Organic semiconductor, CSA doped PANI as a gate electrode, and cross- linked pentaerythrito triacrylate (PETA) as a gate insulator	Activation, Estrogen	1182 Increase, Cell 1193 N/A, Brea Proliferation (Epithelial Cancer Cells)	Acute toxic (Oral) Cat. 4 Skin corrosion/irritation Cat. st 2 Serious eye damage/eye irritation Cat. 2 Skin sensitization Cat. 1	N/A	N/A	Class 4 the fourth petroleum (6,000 L)	N/A
31	Perfluorooctane sulfonic acid	1763-23-1	Photomicrolithograph y	1181 hActivation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cancer Cells)	Flammable liquid Cat. 2 Acute toxic (Oral) Cat. 4 Acute toxic (inhalation: gas) Cat. 4 Acute toxic (inhalation: dus/mist) Cat. 4 Acute toxic (inhalation: dus/mist) Cat. 4 Serious eye damage/eye  strintation Cat. 2 Carcinogenicity Cat. 2 Reproductive toxicity Cat. 1 B Specific target organ toxicity (Repeated exposure) Cat. 1 Chronic aquatic toxicity Cat. 1		N/A	N/A	N/A
32	Phenol	108-95-2	Chip assembly, Mole etc.	1181 Activation, Estrogen receptor	1182 Increase, Cell 1193 N/A, Brea Proliferation (Epithelial Cancer Cells)	Acute toxic (Oral) Cat. 3 Acute toxic (dermal) Cat. 3 Acute toxic (inhalation: dust/mist) Cat. 3 Skin corrosion/irritation Cat. 1 st serious eye damage/eye irritation Cat. 1 Germ cell mutagenicity Cat. 2 Specific target organ toxicity (Repeated exposure) Cat. 2 Chronic aquatic toxicity Cat. 2	management Chemicals for special health exam. (Each 12 months) Chemicals for special	Toxic Chemicals for accident prep.	N/A	Designated waste

33	Piperazine	110-85-0	Chip assembly, Rear Grinding	1181 Activation, Estrogen receptor	1182 Increase, Cell 1193 N/A, Brea Proliferation (Epithelial Cancer Cancer	Acute toxic (Oral) Cat. 4 Acute toxic (dermal) Cat. 4 Skin corrosion/irritation Cat. 1 Serious eye damage/eye irritation Cat. 1 st Respiratory sensitization Cat. 1 Reproductive toxicity Cat. 2 Specific target organ toxicity (Single exposure) Cat. 2 Specific target organ toxicity (Repeated exposure) Cat. 1	,	N/A	N/A	N/A
34	Potassium dichromate	7778-50-9	Photocatalytic reduction using UV radiation and ZnO semiconductor catalyst has been investigated using potassium dichromat as the model Compound	1181 Activation, Estrogen receptor	1182 Increase, Cell 1193 N/A, Brea Proliferation (Epithelial Cancer Cells)	Oxidizing solids Cat. 2 Acute toxic (Oral) Cat. 3 Acute toxic (dermal) Cat. 4 Acute toxic (inhalation: gas) Cat. 2 Acute toxic (inhalation: dus/mist) Cat. 2 Serious eye damage/eye irritation Cat. 2 Respiratory sensitization Cat. 1 Germ cell mutagenicity Cat. 1B Carcinogenicity Cat. 1A Reproductive toxicity Cat. 1B Specific target organ toxicity (Repeated exposure) Cat. 1 Acute aquatic toxicity Cat. 1 Chronic aquatic toxicity Cat. 1	management Chemicals for exposure limits Chemicals for acceptance criteria Chemicals for	Toxic Restricted chemical	Class 1: Dichromic acids (1000 kg)	s Designated waste
35	Tetrachloroethylene	127-18-4	Mold, Chip adhesion Chip assembly, Testing	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cancer Cells)	Skin corrosion/irritation Cat. 2 Carcinogenicity Cat. 1B st Specific target organ toxicity (Single exposure) Cat. 3 (Narcotic effect) Chronic aquatic toxicity Cat. 2	Chemicals for management Chemicals for special health exam. (Each 12	Toxic Restricted chemical	N/A	Designated waste
36	Tetramethyl ammonium hydroxide		Wafer processing, Chip assembly, Photo (developer), Rear tegrinding	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells)	Acute toxic (Oral) Cat. 2 Acute toxic (dermal) Cat. 1 Skin corrosion/irritation Cat. st 1 Serious eye damage/eye irritation Cat. 1 Chronic aquatic toxicity Cat. 2	exposure limits	Toxic	N/A	Designated waste
37	Toluene	108-88-3	Chip assembly, Mole etc.	1181 "Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cancer Cells)	Flammable liquid Cat. 2 Skin corrosion/irritation Cat. 2 Reproductive toxicity Cat. 2 st Specific target organ toxicity (Single exposure) Cat. 3 (Narcotic effect) Specific target organ toxicity (Repeated exposure) Cat. 2 Aspiration hazard Cat. 1	management Chemicals for special health exam. (Each 12 months)	Toxic Chemicals for accident prep.	Class 4 the first petroleum (Insoluble) (200 L)	Designated waste
38	Trimellitic anhydride	552-30-7	Semiconductor assemblies having electrophoretically insulated vias	1181 Activation, Estrogen receptor	1182 Increase, Cell Proliferation (Epithelial Cells) 1193 N/A, Brea Cancer	Serious eye damage/eye irritation Cat. 1 Respiratory sensitization Cat st 1 Skin sensitization Cat. 1 Specific target organ toxicity (Single exposure) Cat. 3 (Respiratory irritation) Acute toxic (Oral) Cat. 4	Chemicals for exposure limits	N/A	N/A	Designated waste
39	Zinc chloride fume	7646-85-7	Semiconductor Manufacturing	Activation, Estrogen receptor	1182 Increase, Cell 1193 N/A, Brea Proliferation (Epithelial Cancer Cells)	Serious eye damage/eye irritation Cat. 1 st Germ cell mutagenicity Cat. 2 Acute aquatic toxicity Cat. 1 Chronic aquatic toxicity Cat. 1	Chemicals for exposure limits	Toxic	N/A	Designated waste

40	Nitric oxide (Nitrogen monoxide) 10102-43-9	Wafer processing, Diffusion	1632 Increase in reactive oxygen and nitrogen species (RONS)	1492 Tissue resident	Cancer	Oxidizing gas Cat. 1 Compressed gas Acute toxic (inhalation: gas) Cat. 2 Specific target organ toxicity (Single exposure) Cat. 1	special health	Chemicals for accident prep.	N/A	N/A
41	Nitrogen trifluoride 7783-54-2	gas used as a cleaning agent for semiconductor and LCD manufacturing	in reactive oxygen and nitrogen species (RONS)	1492 Tissue resident	1193 N/A, Breast Cancer	Cat. 4  Specific target organ toxicity	For Process safety management (PSM) Chemicals for exposure limits	N/A	N/A	N/A